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Groundwater Management Strategy for Michigan Groundwater Modeling: Selection, Testing and Use. Volume 2. Appendices

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Volume 2 Appendices

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B. Investigation of Contaminant Transport Parameters in Michigan Aquifers by S.J. Wright.

C. Aquifer Dispersivities from Field Data - Contaminant Transport in Michigan Aquifers by S.J. Wright

D. Finite Element Modeling of Contaminant Transport by D.C. Wiggert

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by

David A. Hamilton

Task 20 of Groundwater Management Strategy for Michigan
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Water Management Division

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D. Wiggert: Finite Element Modeling of Contaminant Transport

SECTION VII

APPENDICES

APPENDIX A

Southwest Ottawa County Landfill - Assessment of Two-Dimensional Flow Model

by

D. C. Wiggert

MICHIGAN STATE UNIVERSITY

COLLEGE OF ENGINEERING
DEPARTMENT OF CIVIL AND SANITARY ENGINEERING

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June 4, 1982

MEMORANDUM

TO: D. A. Hamilton

FROM: D. C. Wiggert

SUBJECT: Southwest Ottawa County Landfill:
Assessment of Two-Dimensional Flow Model

Your preliminary report outlines a methodology of two-dimensional modeling for the landfill. Both a regional and local model scale have been utilized. The main difficulty encountered was the mound under the borrow area, where the locally predicted piezometric surface did not correlate with the observed values. The field data was vertically averaged for purposes of comparison with the AQUIFEM model. The predicted results appear to be quite satisfactory in light of the complexity of the system and the available field data.

Some three-dimensional effects have been observed in the contaminant plume delineated by resistivity measurements. In attempting to locate a purge well system in proximity to the landfill, you are proposing to make use of the two-dimensional flow model AQUIFEM coupled with ongoing field measurements to optimize placement of the wells. Specific aspects of your methodology include: assigning confining layers or raised bottom elevations to account for lenses, vertically averaging the piezometric head, and additional two-dimensional interpretation of field data. At some distance away from the site (say about 0.5 mile) it is likely that most of the three-dimensional effects will have disappeared, and that a two-dimensional flow assessment will provide sufficient accuracy.

By continuing field investigations you will gain more knowledge with regard to the local aquifer properties and conditions. As a result, the AQUIFEM model can be periodically updated and improved upon to yield more precise predictions. It appears that you have obtained sufficient three-dimensional data to produce an acceptable two-dimensional prediction. Additional data that would be useful includes more precise locations of lenses and their properties, and further measurements of the piezometric gradients -- both horizontally and vertically -- to better delineate flow movement and boundary conditions.

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I do not believe it is worthwhile to attempt to use a three-dimensional flow model. A major obstacle in such modeling is the necessity to obtain sufficient data to effect accurate predictions. Since such data procurement is time consuming, difficult and costly, it is usually incomplete. As a result, the modeling uncertainties remain high, and the resulting predictions may be no more meaningful than the two-dimensional predictions based on vertically averaged parameters.

The two-dimensional methodology used at the Southwest Ottawa site should be applicable to similar sites. The knowledge gained from the present study should make it possible to investigate future sites with improved efficiency, e.g., selecting the minimum requirements for field data, increased confidence in the modeling predictions, and optimum placement of purge well systems.

DCW/nlh

APPENDIX B

Investigation of Contaminant Transport Parameters in Michigan Aquifers

by

S. J. Wright

INVESTIGATION OF CONTAMINANT TRANSPORT PARAMETERS IN MICHIGAN AQUIFERS

BY

STEVEN J. WRIGHT

PROJECT REPORT

TO

MICHIGAN DEPARTMENT OF NATURAL RESOURCES

JULY 1, 1981

INVESTIGATION OF CONTAMINANT TRANSPORT PARAMETERS IN MICHIGAN AQUIFERS

INTRODUCTION

This report describes the preliminary results of an investigation into contaminant transport processes at selected locations within the state of Michigan. The primary purpose was to determine parameter values used to describe the hydrodynamic dispersion processes at specific locations with existing contamination problems. An additional objective was to examine the adsorption characteristics of specific contaminants. Previously obtained field data was analyzed in order to accomplish these objectives.

Two sites were selected in the preliminary phase of the investigation: 1) A styrene spill from a train derailment near Pearl, Michigan in May 1979; 2) Contamination resulting from waste disposal practices at Ott/Story Chemical Company near Muskegon, Michigan. The Pearl site is characterized by a one time spill with subsequent attempts at a cleanup of the styrene that was released. All pertinent information regarding data collected at that site has not been received at the present point in time and only a preliminary analysis has been made; the final project report will deal with this site in more detail. It presently appears that the "local" nature of the problem

will make it difficult to obtain a meaningful analysis. Additional complications arise because of the tendency for styrene to polymerize and be retained in the unsaturated zone only to enter the groundwater system after rises in the groundwater table.

The Story Chemical site analysis has been more tractable and the remainder of this report deals with this subject. The contamination apparently resulted primarily from seepage from waste lagoons on-site during the 1960's and 70's. The wastewater contained relatively high concentrations of chloride ions in addition to a number of organic compounds. Large enough concentrations of contaminants have apparently entered the water table aquifer to have some density effect since the highest contaminant concentrations are found at or near a clay layer serving as an effective bottom to the aquifer. However, no indication is present that this influence has been important in determining the migration routes of the contaminants. The chloride data have been used in the analysis of aquifer dispersivities because of their relative abundance and the fact that chloride ions are not significantly adsorbed in the soil matrix. Analytical procedures are used to obtain estimates of the aquifer dispersivities and the resultant values are used in a numerical solution of the groundwater flow at the site to provide additional verification. Data on specific organic chemicals is also examined to attempt to define adsorption characteristics in the

aquifer system. These results are presented herein along with interpretations justified within the uncertainty of the available data.

DATA BASE

A number of different sources of information were obtained from the Michigan Department of Natural Resources files. These include the following reports or other sources of information:

1. Williams and Works Engineering report to the Ott Chemical Company, Nov. 1966 entitled "Water Supply and Waste Water Disposal."

2. Miscellaneous data provided by Williams and Works to the Ott Chemical Company providing interpretation of groundwater quality samples at or near the company location. These are in the form of contour plots of phenol and chloride concentrations and range in time from 1971 to 1975.

3. A report entitled "Report of Groundwater Quality and Storage of Wastes at Story Chemical Corp., Muskegon, Michigan based on a survey conducted March 8-9, 1977." Concentrations of various chemicals at selected observation wells are included in this report which is assumed to have been produced by the D.N.R.

4. Portions of a report by Keck Consulting Services to the DNR entitled "Hydrogeological Investigation, Story Chemical Company, . . ." November 10, 1977. This includes chloride concentrations at various observation wells from 1965 to 1977.

5. Summary sheets of water quality data from the Muskegon County Health Department obtained July and August, 1977. Various chemical parameters are analyzed.

6. D.N.R. report entitled "Hydrogeological study of Groundwater Contamination in the Area of the Former Story Chemical Company." This includes sampling with depth at seven observations wells, primarily in 1978.

7. D.N.R. Report entitled "1979 Hydrogeological Study of the Groundwater Contamination in the Area of the Former Story Chemical Company." Results of sampling at various observation wells is presented.

8. Report by Keck Consulting Services to D.N.R. entitled "Ott/Story Chemical Groundwater Contamination Study," September 6, 1979.

9. Ott/Story Chemical Company Hydrogeological Investigation; Phase A-6: Computer Simulation July 3, 1980 and related correspondence to Gary Klepper (D.N.R.) of October 22, 1980 and December 4, 1980.

10. Appendix to previous report "Review of Data: Phase A-4."

While it is probable that there is additional information available regarding hydrogeologic conditions at the site, the above data provides a reasonably continuous record of chloride concentrations in the groundwater aquifer from 1965 to 1980, phenol concentrations from 1975 to 1980, and various other organic chemicals at irregular intervals.

Groundwater levels are provided in various of the above reports and References 8-10 contain information on aquifer characteristics. These data were used to generate the results presented in this report. A previous numerical simulation, (9)*, was performed in which the groundwater flow in the area was computed. This was used as a starting point for the present numerical simulation in which contaminant transport is also included. Changes in the simulation details from the previous report are documented and justified by interpretation of the available data. The major difference in the present approach is the inclusion of the water quality data in the problem interpretation.

CONTAMINATION PLUME ANALYSIS

Since there was considerable information on chloride concentrations in the aquifer, this source provided the most information regarding transport parameters. Although chlorides may be present from additional sources (notably road de-icing operations) the chloride concentrations in the contaminant plume are so large this source is relatively easy to identify compared to other minor fluctuations in background levels. Chloride concentrations in the plume in excess of 2000 mg/ℓ were not unusual compared to background levels of less than 10 mg/ℓ. A considerable number of samples where adjacent observation wells sampled both shallow and

*In the remainder of this report, information referenced is indicated by the numbers assigned above.

deep portions of the aquifer indicated that higher chloride concentrations were found at greater depth. This could be due to either density effects or the natural recharge diluting the near surface waters. In fact, probably both effects are present. Consideration of this fact resulted in a decision to only analyze deep well chloride concentrations since data for shallow observation wells may be distorted by further migration of chlorides towards deeper levels with distance away from the source. On the other hand, concentrations in deep observation wells were relatively large at or near the chemical company site indicating vertical movement was fairly rapid and deep well concentrations should not be affected significantly by three dimensional effects.

Selected plots of chloride contours are presented in Figs. 1-6 for deep observation wells. Sources of data are indicated on the figures which cover the span in time of available information. These data, along with other information available, support the following general conclusions:

A. Early in the time period covered by the data, a substantial amount of the contamination problem was confined to the immediate site. 1965 data appear to indicate a general movement from the waste lagoons to the pumping wells on-site. The effect of pumping on-site seems to have been to deflect the plume somewhat to the southwest.

B. Recharge ponds do not appear to be a significant source of contamination at any point in time.

C. After the mid 1970's, chloride concentrations have been dropping at the upstream end of the plume with the cessation of waste discharge and the aquifer system appears to be flushing itself.

Plots of phenol concentrations for the years of 1975, 1977, and 1979 are given in Figs. 7-9. Since the time record on this data is not as long, it is more difficult to draw conclusions. A critical assumption is that these compounds entered the aquifer system at the same time as the chloride contamination. Inherent in this assumption are the following two considerations; (1) phenol and chloride concentrations in the source were directly proportional to each other and (2) the distance from the source to the water table is short enough that adsorption in the unsaturated zone is not a critical element of this problem. If these assumptions are valid, then the following general conclusions may be made:

Phenolic compounds are relatively strongly absorbed in the aquifer media and are retarded significantly in their horizontal movement. This is evidenced by a buildup in concentrations at the Little Bear Creek tributary only beginning to be evidenced in the late 1970's. Concentrations are still rising relatively close to the site during the time period in question. This contaminant may be expected to persist in the aquifer for a considerable length of time.

The validity of the above conclusions will be further addressed during the presentation of the results of the numerical simulation.

Miscellaneous measurements for other organic chemicals related to the Story Chemical Company operation were investigated to determine their transport in the aquifer system. Sufficient information on benzene, toluene, and aromatic amines was obtained to be able to estimate their distribution; the results are provided in Figs. 10-12. If the same assumptions as made regarding the movement of phenols is made, it is possible to determine their relative adsorption characteristics. In order of relative mobility, aromatic amines appear to be the most mobile with benzene the least. All are more mobile than phenols and may be expected to flush from the system more rapidly. There is such little data that these conclusions can only be regarded as very tentative; they will be discussed later in the presentation of the numerical results. Insufficient data is available on the concentrations of other compounds to be able to draw any general conclusions on their rate of movement in the groundwater system. It can be anticipated that this is due to several factors including: low concentrations of specific compounds; large retardation factors and very little movement with lack of data at the various observation wells; and difficulties with analytical procedure due to the presence of many unknown contaminants.

Additional test results are available for 1978 and 1979 for ammonium ion NH_3^-, but they will not be analyzed in any detail. The very high PH of the contaminated water will likely have a significant influence on the chemistry that may not be repeated at other potential contamination sites. The available data however seem to indicate NH_3 movement with very little adsorption effects in this particular plume.

MODEL FORMULATION

Since the above conclusions are only qualitative in nature, an attempt was undertaken to quantify them as well as fulfill the basic objectives of this investigation. In order to do this, a numerical model was formulated which solved the simultaneous problems of groundwater flow and contaminant transport. The U.S. Geological Survey "Method of Characteristics" program* was selected as the modeling tool because of relative familiarity with its use and some degree of confidence in its ability. Although this program is not formulated to be able to analyze flow with adsorption, it is possible to transform some input parameters and obtain a solution if a linear, reversible adsorption isotherm (i.e. that the use of retardation factors is valid) is assumed. Details are discussed in the following sections. Parameter identification for this model was accomplished by a variety of techniques as outlinedin the following pages. The result

*Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water," by L. F. Konikow and J. D. Bredehoeft, Techinques of Water-Resources Investigations of the U.S.G.S. Chapter C2 Book 7.

is a model that is believed to provide a realistic description of the general aquifer behavior at the Ott/Story Chemical site and allows more specific conclusions regarding the contaminant transport parameters for this location. A more thorough analysis of the problem may well yield a model that better reproduces details of the contaminant migration in the system as this was not the present objective of the model formulation.

Modeling Philosophy

The numerical model was not constructed with the intent of reproducing the observed contamination profiles as closely as possible. Instead, it was used as an aid in sorting out the various influences in the problem and the determination of the appropriate transport parameters. As such, unless additional detail was deemed to be of critical importance to the results obtained, it was not included in the formulation. It is also possible that additional data, known to exist but not available at the time of the model formulation, would alter the specific formulation somewhat. On the other hand, the uncertainty in various details of the actual problem probably renders additional complexity unjustifiable in most instances.

The first attempt was to reconstruct the groundwater flow in the area. The starting point for this part of the simulation was the previous study by Keck Consulting Services (9) and the 1979 data on water table elevations (8).

Adjustments to the previous simulation results were made as outlined and justified in a subsequent section until a reasonable reproduction of the water table levels was obtained. Steady state groundwater flow conditions were assumed throughout the analysis as the only justifiable approach given other uncertainties in the problem resolution. From the groundwater flow model, the contaminant transport model was used to attempt to reproduce the detail of the chloride plume. Only one adjustment as discussed later was made to the initial simulation.

This change was required only because the initial run was known to oversimplify the source detail from the beginning and the final description is one that was visualized as the most appropriate from the outset of the modeling effort. Considerable detail regarding temporal and spatial distribution of groundwater pumping at the site and contaminant discharge is not included in the model. This is because this detail is both not accurately known and not felt to be of critical importance to the assessment of aquifer parameters. On that basis, only one release scenario was investigated; however it is felt to be reasonably consistent with the known detail at the site. Once the contaminant plume simulation was obtained, the effect of retardation on the expected plume behavior was investigated. The sensitivity of the model to the various transport parameters is investigated, and finally, the results obtained are interpreted in light of the available data and appropriate conclusions are drawn.

Parameter Identification

The initial information on the groundwater flow portion of the problem were taken from the previous numerical simulation by Keck Consulting Services (9). Specifically, these are tabulated in Table 1 along with the source for the parameter estimate. The saturated thickness of the aquifer for the present simulation was taken as 70 ft from the well

Table 1 - Hydraulic Parameters for Local Aquifer

Parameter	Estimated Value	Source
Hydraulic Conductivity	66.8 ft/day	small scale pump tests described in (10)
Specific Yield	0.1	estimate
Local Groundwater Recharge	10 inches/year	estimate from (4)
Specified piezometric head boundary conditions	variable	water table contours from previous hydro-geologic invesitgation (4)

log data given in (8). The discussion of the Keck numerical solution provides additional detail on this. Of the above parameters in Table 1, only the groundwater recharge rate was kept as in the previous simulation. Since no better estimate of this rate was available, it was not considered

to be a variable subject to analysis. The additional parameters were adjusted as deemed necessary, but still consistently with available information. The small scale pump tests conducted by Keck Consulting Services (10) were at such low flow rates that the storativity coefficient was more nearly due to that of a confined aquifer situation when the well logs clearly indicate an unconfined aquifer. This behavior is often noted for small drawdowns in water table aquifers and requires a longer pumping time to make an accurate assessment of the actual specific yield. The pump test results were interpreted by assuming an effective aquifer thickness of the screen length of the pumping well and dividing the computed transmissivity by that length to obtain hydraulic conductivity. In actuality, the vertical distance influenced by the pumping will be greater than the screen length, so a somewhat lower hydraulic conductivity than the value in Table 1 would be expected. Previous studies cited in (9) gave hydraulic conductivities of between 20 and 60 ft/day and support the above conclusion. No estimate was available for the specific yield, but it is understood that the value of 0.1 was selected on the basis that it provided a conservative estimate or "factor of safety" in the results obtained from the numerical simulations. A further attempt to rationalize the values of these two parameters

was obtained from the chloride concentration profiles (2) and the time of travel of the chloride peaks. Although this procedure is suspect due to the lack of resolution in chloride data, it did point out some inconsistencies in the previous parameter values. The Darcy velocity could be estimated from the local hydraulic gradient given by $q = K \Delta\phi/\Delta\ell$ and the seepage velocity by

$$V = \frac{\Delta\ell p}{\Delta t}$$

Here K is the hydraulic conductivity, $\Delta\phi/\Delta\ell$ is the water table slope obtained from the contours given, $\Delta\ell p$ is the distance the concentration peak moves in time Δt. Nearly all of these calculations clearly indicate a specific yield $Sy = q/V$ much greater than physically expected. Figure 13 indicates a sample calculation. A specific yield of 0.73 is much greater than can be physically expected. The difficulty now is that the determination of K and Sy cannot proceed independently from these data since a reduction in K will produce a proportional reduction in Sy. Subsequently, a value for Sy of 0.25 was assumed and a hydraulic conductivity of 32 ft/day was estimated. The approach was to take as large a value of specific yield as physically realistic and determine what hydraulic conductivity would give a good match between the Darcy and seepage velocities.* This approach may

*Note the recent report "Management Options Contaminated Ground Water Plume Ott/Story Chemical Company" by Keck Consulting Services and Snell Environmental Group Inc., June 1981, estimates a larger specific yeild than 0.1 and also notes the possibility of a lower hydraulic conductivity.

be subject to considerable question, but the reduction of hydraulic conductivity appeared to give a much better simulation of water table levels as discussed later. These values were used without modification in the numerical simulation. The transverse dispersivities were also estimated from the same data on chloride profiles. There was never adequate enough resolution of the leading edge of the plume to attempt an estimate of the longitudinal dispersivity so in all analyses a value three times that of the lateral dispersivity was assumed. This approach is simply consistent with known variations of the two components from previous studies. The lateral dispersivity was estimated by an analytical procedure which requires a large number of assumptions:

Molecular diffusion effects are negligible;

Steady release of a point source of contaminant;

Two dimensional contaminant transport;

Negligible longitudinal dispersion;

Uniform ground water flow.

Of the above, the second and last are the most critical assumptions for the specific problem, but the effect of these influences was mitigated by the approximate procedure used. For the above assumptions, the lateral concentration profile is given by

$$C = C_{max}\, e^{-y^2/4\alpha_T x}$$

where y is lateral distance from the peak concentration C_{max}, x is longitudinal distance from the source, and α_T is the transverse dispersivity. Then by definition

$$\sigma^2 = 2\alpha_T x$$

where σ^2 is the variance of the lateral concentration distribution. The effect of the point source approximation is removed by taking the derivative

$$\frac{d\sigma^2}{dx} \approx \frac{\Delta\sigma^2}{\Delta x} = 2\alpha_T$$

and observing the rate of growth of the plume width. The uniform flow assumption is partially negated by measuring distance along the plume travel path. The concentration profiles taken directly from (2) between 1974 and 1975, a plume profile in 1976 from (4) and the present estimate of the plume location ((9), correspondence of October 22, 1980) were used to estimate the transverse dispersivity. In all cases except the last, a Gaussian profile was approximated through the plume data, and a total width of 4σ was estimated. In the latter case, a width of 4σ for the plume outline was assumed. This procedure was repeated for two or three locations along the plume and corresponding values of α_T were computed. Figures 14-16 demonstrate example calculations and Table 2 summarizes the computed results. From these data, a value for α_T of 20 ft was estimated

Table 2. Estimates of Lateral Dispersivity
(distances in ft)

Date (source)	X_1	X_2	σ_1	σ_2	α_T	Average
Nov. 1974	1070	1860	200	275	22.5	20.5
(2)	1860	2670	275	325	18.5	
May 1974	1160	1740	250	295	21.1	18.8
(2)	1740	2760	295	350	17.4	
Jan. 1975	1290	2275	230	288	15.3	18.1
(2)	2275	3140	288	346	21.3	
1976 (4)	700	2650	275	400	21.1	
1980 (8)	1415	3200	350	450	22.4	
					Average	20.2

with only a small amount of scatter in the computed results. This value and a longitudinal dispersivity of 60 ft were taken as the baseline values in the numerical simulations although a sensitivity analysis was performed. These values are consistent with previously reported values for similar aquifer systems* and so are presumed to be fairly reliable estimates for those parameters. A retardation factor was only estimated for phenols since that was the compound for which the most data was available and also since it appeared to be the least mobile of the specific chemicals investigated. Only a crude estimate of the retardation factor was obtained and used in the numerical solution to observe its influence. The considerations involved in this analysis were as follows:

According to (4), little chloride movement off site was detected in 1965. This would place the beginning of the plume migration problem some time in the middle to late 1960's. Assume phenols were present in the initial waste discharge. By 1975 they have shown high concentration (17 mg/ℓ) in observation well 17 (Fig. 17) and continue upwards to values of 22 mg/ℓ in 1977 and 38 and 43.5 mg/ℓ in 1979. In 1980 levels of 27 mg/ℓ were detected, indicating peak concentrations have possibly arrived at the site. On the other hand values of only

*J.J. Fried "Groundwater Pollution," Developments in Water Science," Volume 4, Elsevier Publishing Co., 1975.

3 or 4 mg/ℓ are detected further downgradient at observation wells A & C in 1978 and 1979. Chloride levels were high in well 17 in 1968 and never got much larger than that. From this, the relative time of movement to well 17 could be approximately 5 years for chloride and perhaps 15 years for phenols, giving a retardation factor of approximately 3. This value would give a time of movement for peak concentrations of perhaps 30 years or more to observation wells A and C. This value of retardation factor was used in the numerical model discussed later to observe whether results consistent with the observed data could be generated.

NUMERICAL SIMULATIONS

A series of numerical simulations were performed to obtain some additional information regarding the transport parameters at the Ott/Story Chemical Company Site. Basically the approach was similar to that used in the previous simulation by Keck Consulting Services (9). The grid with 400 ft spacing between nodes was used in the simulation effort to be consistent with the previous analysis.

WATER TABLE SIMULATIONS

Specified head boundaries were applied at all exterior nodes (actually one node in from the boundary as shown in Fig. 18) and along Little Bear Creek and tributary as in

Fig. 19. Most of the boundary nodes are far enough removed from the contamination site that a significant change in boundary head only influences the interior heads a relatively minor amount. Calculations are much more sensitivie to the heads specified along the creeks and these represent a critical element of the simulation. The U.S.G.S. model has the capability of performing a steady state computation with only boundary heads specified. In this procedure, all interior heads are left unspecified and are computed in the simulation. The interior water table elevations so computed were then compared to available water level observations (8). One difficulty with the available data is that there were two types of observation wells; one with screens at depth and another which sampled the water table location directly. There appears to be a significant component of vertical flow as adjacent wells show approximately 1.6 ft difference in head between deep and shallow observation wells at a considerable distance from the creek. Scatter in water levels essentially adjacent to the creek indicate that significant vertical velocity components must exist and therefore large changes in head with depth. Interpretation of the available data becomes difficult near the creek which is unfortunately the most critical area from the standpoint of supplying boundary conditions. An initial head distribution along the creek was selected however as given in Fig. 20 and never altered during subsequent calibration attempts.

Initial runs with a hydraulic conductivity of 66.8 ft/day yielded results that appeared to predict piezometric heads too low at the interior locations of the grid. Lowering the hydraulic conductivity to 32 ft/day raised interior heads by approximately 1.5 ft and yielded much more satisfactory water table comparisons. On the basis of this and the previous discussion, the lower value of hydraulic conductivity is recommended for future simulations. The final simulation selected gave the groundwater contours shown in Fig. 21, and yield as good as an agreement with the available data as appears reasonable to expect. This basic data was then used in all further simulations of the site.

CONTAMINANT PLUME SIMULATIONS

After much consideration of the possible source descriptions, a somewhat simplified approach was taken. This is again consistent with the modeling philosophy of transport parameter simulation and does not reflect accurate histories of contaminant plume movement. Future simulations for management decisions, should they be performed, may want to consider better descriptions of the source. It was decided that the two most important considerations were probably source location and the influence of pumping at the site. The U.S.G.S. model offers the alternatives of concentrating contaminants at a point (injection well) or over a grid cell

which in this case is 400 ft square. Since this is on the order of the size of the original waste ponds, the latter option was used and a single node slightly downgradient of the actual ponds was used as the source location. Its position is indicated in Fig. 19. A source concentration of 3000 (arbitrary units) was used to check chloride concentration profiles since this is representative of maximum chloride concentrations in mg/ℓ observed. The Williams and Works data (2) seem to indicate a drop in chloride concentrations near the source in the early 1970's and a gradual decrease continues over time. The source was assumed to be in effect for 10 years (e.g. from 1958 to 1968 or some similar description) and then completely removed thereafter. Although it is known that the contamination continued after that point, the relative amounts of contamination input in the two periods is unknown and it was primarily desired to observe the computed plume movement. Again, this description could be criticized for various reasons but there seems to be some merit in such a description. Finally, rather than attempt to specify recharge and pumping rates at the Story Chemical site directly, specified heads were used as source conditions. The Williams and Works data (1) indicate an approximate 1 ft rise in head below the waste ponds and drawdowns of up to 8 or 9 feet below that level at nearby pumping wells. The effect of pumping wells was included in a crude sense only because the early data seemed to show

that the contamination moved in response to pumping and migrated more to the southwest than otherwise expected. Pumping wells were assumed at two nodes as indicated in Fig. 19 and heads of 9 ft lower than that below the waste ponds were specified. The waste pond head was determined by taking the result of the water table simulation at that node and simply adding 1 ft to it. After the initial 10 year period, the construction of the recharge ponds on site appparently effectively stopped the pumping well influence, so these effects were removed from the simulation after 10 years. Again, it should be emphasized that these steps were performed because a great deal of source information was not available and only the qualitative effects of the source were felt necessary to examine transport parameters. It should be mentioned that the above description was selected in advance of any model calibration attempts and does not represent any attempt to reproduce the plume location or behavior.

RETARDATION EFFECTS

The effects of absorption were included in the numerical solution to examine movement of some of the other chemical compounds in the aquifer. Although the U.S.G.S. model does not include adsorption effects, this can be included in a relatively straight forward manner. The general equation

for contaminant transport as solved by the U.S.G.S. program is

$$\frac{\partial C}{\partial t} = - \nabla \cdot (\frac{q}{n} C) + \nabla \cdot (D_h \nabla C) + S_o$$

i.e. no chemical reaction or adsorption terms are given. Here C is contaminant concentration, q is the specific discharge vector, n is the effective porosity, D_h is the hydrodynamic dispersion tensor, and S_o represents sources or withdrawals of fluid. If the adsorption process is considered to be given by a linear reversible isotherm, the above equation is modified by multiplying the time derivative term by a retardation factor R_d.* Since we don't have any information to the contrary, this approach is assumed in this study. Dividing all sides of the equation by R_d implies that if the effective porosity is multiplied by R_d and the dispersion coefficient is divided by R_d, all flow terms in the above equation will be adjusted properly to account for adsorption. Also, it is important to note that the U.S.G.S. program uses a separate term for aquifer storativity and effective porosity so no conflict arises in the solution of the flow equation. Since a recharge rate is not being directly specified in the numerical simulation, the source term S_o is not modified and the amount of water

* "Hydraulics of Groundwater," J. Bear, McGraw Hill Inc., 1979.

entering the system is the same in an adsorbing and non-adsorbing case.

PLUME SIMULATION RESULTS

An initial set of runs was performed to investigate the sensitivity of the lateral dispersivity in the solution relative to the source description. A baseline run with no pumping well effects was run for a simulation period of 8 years with the contaminant source located as discussed previously. The lateral and longitudinal dispersivities were taken to be 20 and 60 ft respectively. Additional runs with the dispersivities doubled and halved; a comparison of the results is given in Fig. 22 in which the location of the 100 (corresponding approximately to mg/ℓ of chloride) contour is plotted. It can be seen that the groundwater mounding at the source provides a relatively rapid initial spreading and dispersion effects downgradient are more or less as expected; higher coefficients give greater plume extent. A similar run with the simulated effect of pumping included as previously described and the original dispersivities is indicated in Fig. 23. The major conclusion to be drawn from Figs. 22 and 23 is that determination of α_T by comparison with the plume extent by means of a numerical simulation is not likely to be very adequate. The difficulty is that the source details apparently have a much larger influence on the plume extent than do the magnitude of the dispersivities

within a reasonable range of their variation. From this, it is recommended that the original value of 20 ft for the lateral dispersivity be accepted as a best estimate for the site in question until such time as better evidence may become available.

With the above considerations, the plume simulation was continued in time with the source detail outlined previously. Figures 24-26 give details of the plume profiles for times of approximately 10, 15 and 20 years respectively. Included for comparison sake is information of the actual plume detail estimated for 1968, 1973, and 1978-79 which are felt to be roughly corresponding points in the time history of the plume development. Results of these comparisons are quite reasonable although it is clear that an altered description of the source detail could probably resolve the plume location better in the vicinity of the chemical plant site. In particular, the removal of the source at t = 10 years is obviously in error as the simulated plume has moved nearly off site by the end of 20 years. A more nearly correct simulation would be to continue the source after 10 years with some reduced concentration level without influence of on site pumping included.

The most significant discrepancy between the numerical and measured plume profiles is the lack of agreement between the two on the location of the northeastern plume boundary.

It would be easy to advance the argument that so little observation well data is available in the vicinity of the plume boundary that the lack of agreement is due to insufficient field data. However, it is also realistic to expect that this discrepancy is real and due to the specified heads along the Little Bear Creek tributary in the numerical solution. The computed groundwater profile in this vicinity seems to agree very well with the 1979 water level data presented in Fig. 21 but is should be noted that the previous simulation by Keck (9) would have resulted in a plume deflected more to the south as it enters Little Bear Creek and Tributary, as indicated by Fig. 27 which was a run made in early 1981 without all the detailed information now available. Basically, Fig. 27 reproduces the Keck groundwater flow simulation with a source at the location indicated and no pumping well influence. The correct description of the groundwater flow in this vicinity may well lie in between the two simulations, but the present approach locates the plume boundary more adequately.

The effect of contaminant retardation was studied by comparison with the phenol data. A retardation factor of 3 was used in the simulation as previously estimated. The results of simulations are presented for 10, 15 and 20 year periods in Fig. 28-30. For comparison, phenol data from 1975-79 are included in Figs. 29 and 30. Since the contaminant has not moved as rapidly in this case due to

adsorption, details of the source become much more critical Given the lack of detail presently incorporated in the numerical simulation, a surprisingly good agreement is obtained. The important conclusion is that a retardation factor of 3 seems to be realistic for this particular compound in the given aquifer system. A detailed investigation for the other parameters (benzene, toluene, and aromatic amines) was not conducted due to lack of detailed data, but it is relatively clear that their retardation factors should be corresponding smaller. This can be incorporated into a later phase of the present investigation if desired.

The phenol simulation was extended in time beyond the present to estimate the flushing from the aquifer system under natural conditions. Note that the contamination was turned off in this simulation at an approximate date of 1968 when it actually is known to continue up through the middle 1970's to some extent. The 1 mg/ℓ (approximately estimated by comparison of maximum phenol concentrations observed in Fig. 7-9 with computed values) contour is shown to develop in time in Fig. 31. The obvious implication of the 15 year maximum flushing time estimated (9) for this site has very little to do with the persistence of chemical constituents in the present aquifer as the retarded pollutant plume is barely "reaching" the Little Bear Creek tributary after this time. An estimated natural flushing time for

phenolics would be more on the order of 50 years, provided that reasonable estimates regarding the pollutant behavior has been made in this study. It must also be considered likely that other chemical constituents have been more strongly adsorbed than the ones investigated. There are some rather significant consequences with respect to management options on site cleanup inherent in these results.

CONCLUSIONS

The numerical model and simulations described herein were not intended to develop detailed description of the plume behavior, but comparisons of actual data appear to yield surprisingly good agreement with the numerical results. Therefore, with some minor modifications of the source description, it is felt that this model could be used to evaluate management options presently under consideration at the site. The results of this study have produced the following conclusions:

1. A realistic estimate of the lateral dispersivity is 20 ft for the sand aquifer in question. Available data seems to be in strong support of this value.
2. No information could be generated to estimate the longitudinal dispersivity directly, but the comparison of the phenol data with the corresponding numerical simulation lends support for the value of 60 ft adopted.
3. A retardation factor of approximately 3 appears to be appropriate for the adsorption of phenols in this aquifer.

4. Retardation factors lower than that for phenols would be required to describe the apparent movement of benzene, toluene, aromatic amines, and ammonium through the aquifer. The latter two appear to be subject to negligible adsorption in the contamination plume. Benzene appeared to be more strongly absorbed than toluene but an insufficient data base prohibits determinations of retardation factors with any degree of confidence.
5. Adjustments to the previous numerical simulation of groundwater flow at the site appear to be necessary to yield satisfactory agreement between the observed and computed plume detail.
6. Long natural "flushing" times for the aquifer in excess of 100 years may be expected for some of the organic chemicals present.

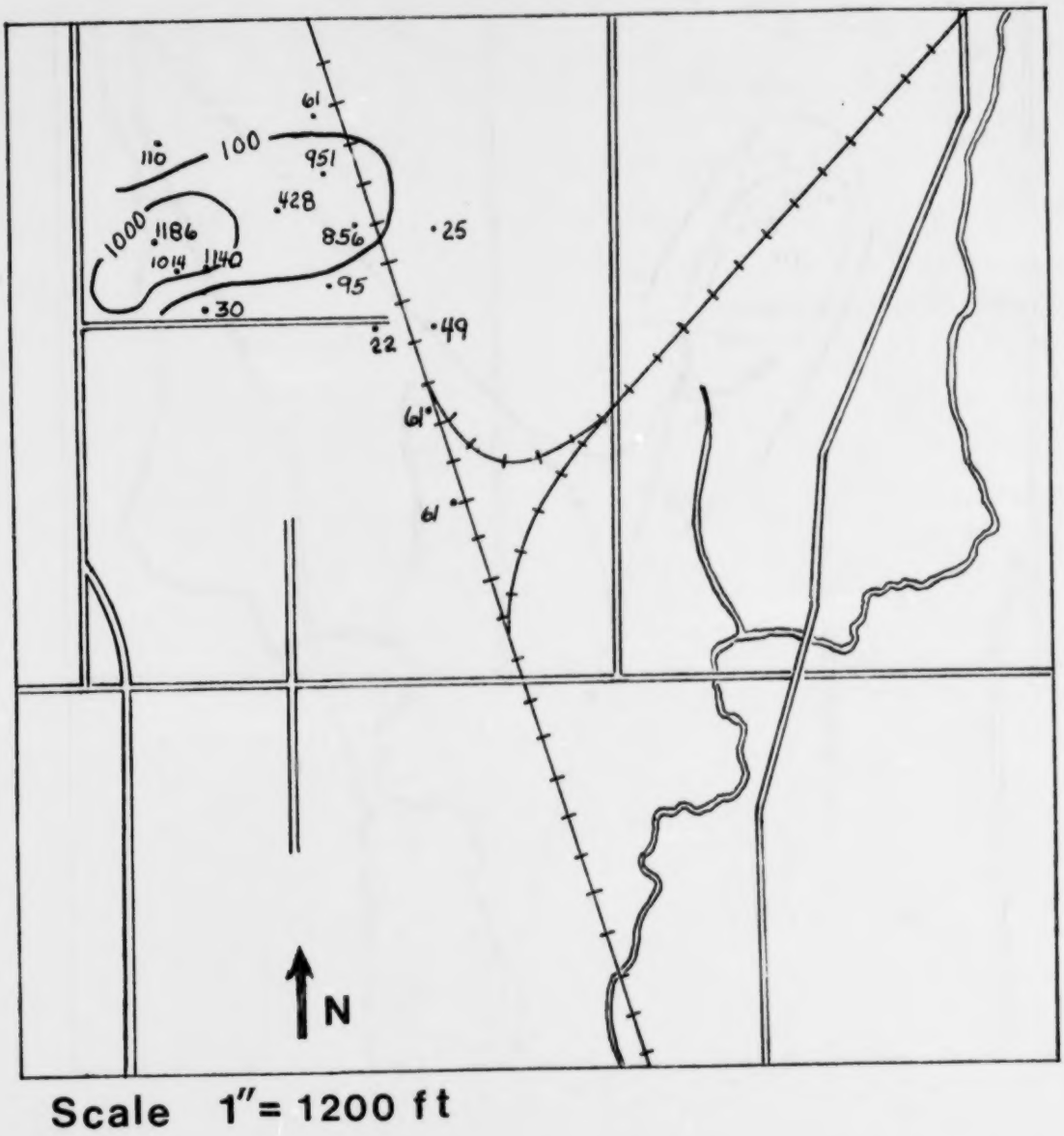


Figure 1. 1965 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from Keck (4).

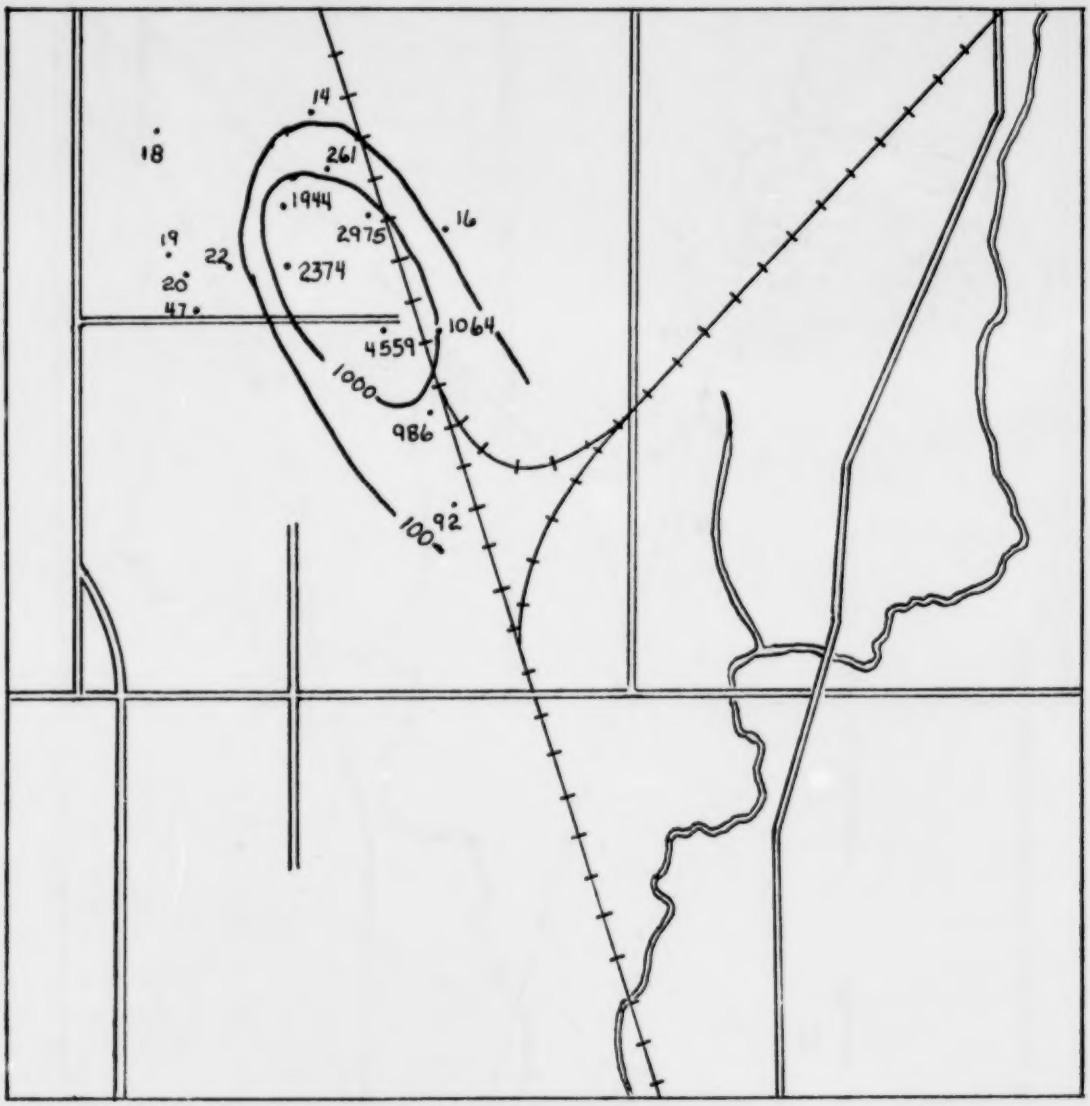


Figure 2. 1968 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from Keck (4).

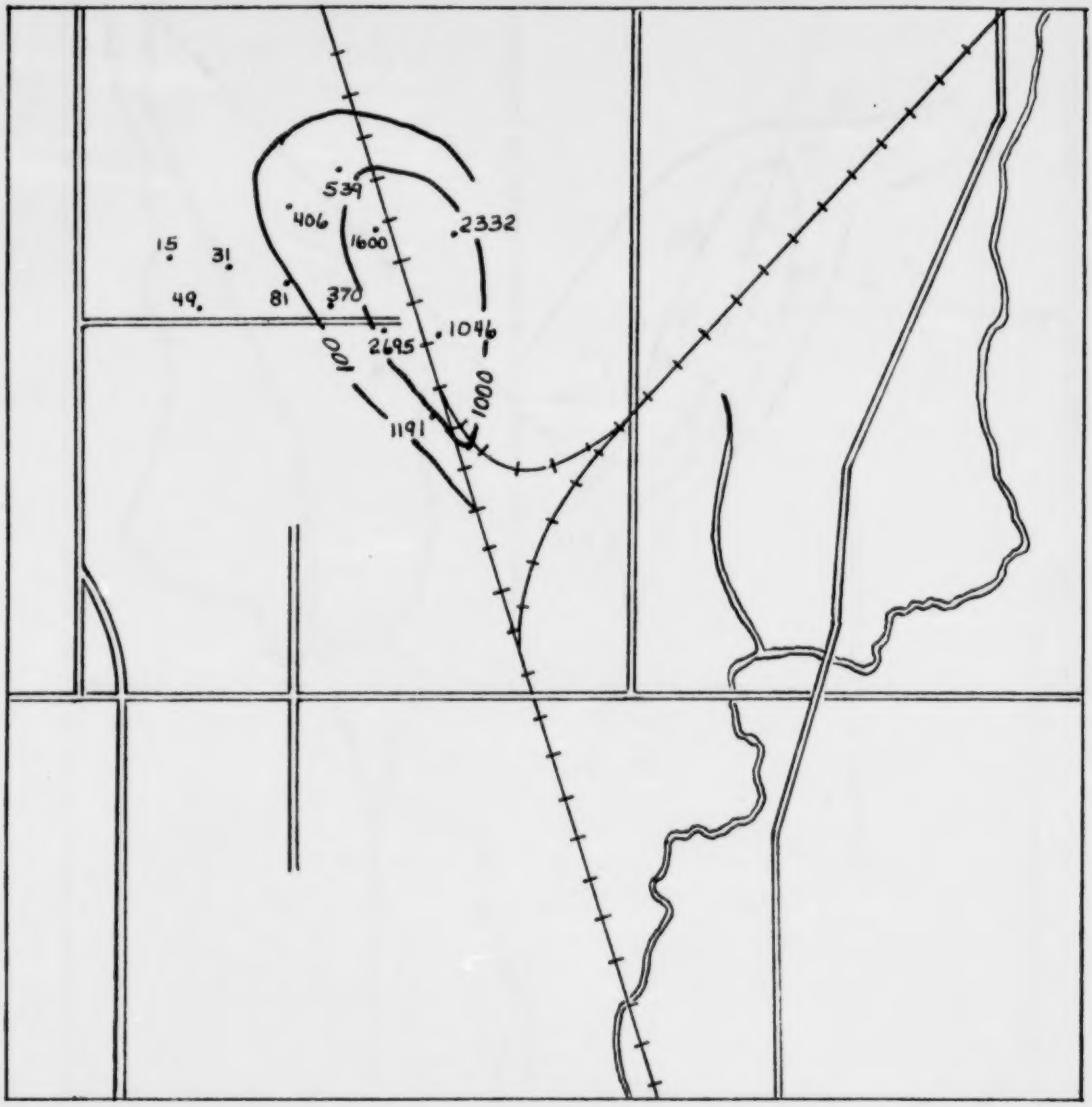


Figure 3. 1971 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from Williams and Works (2).

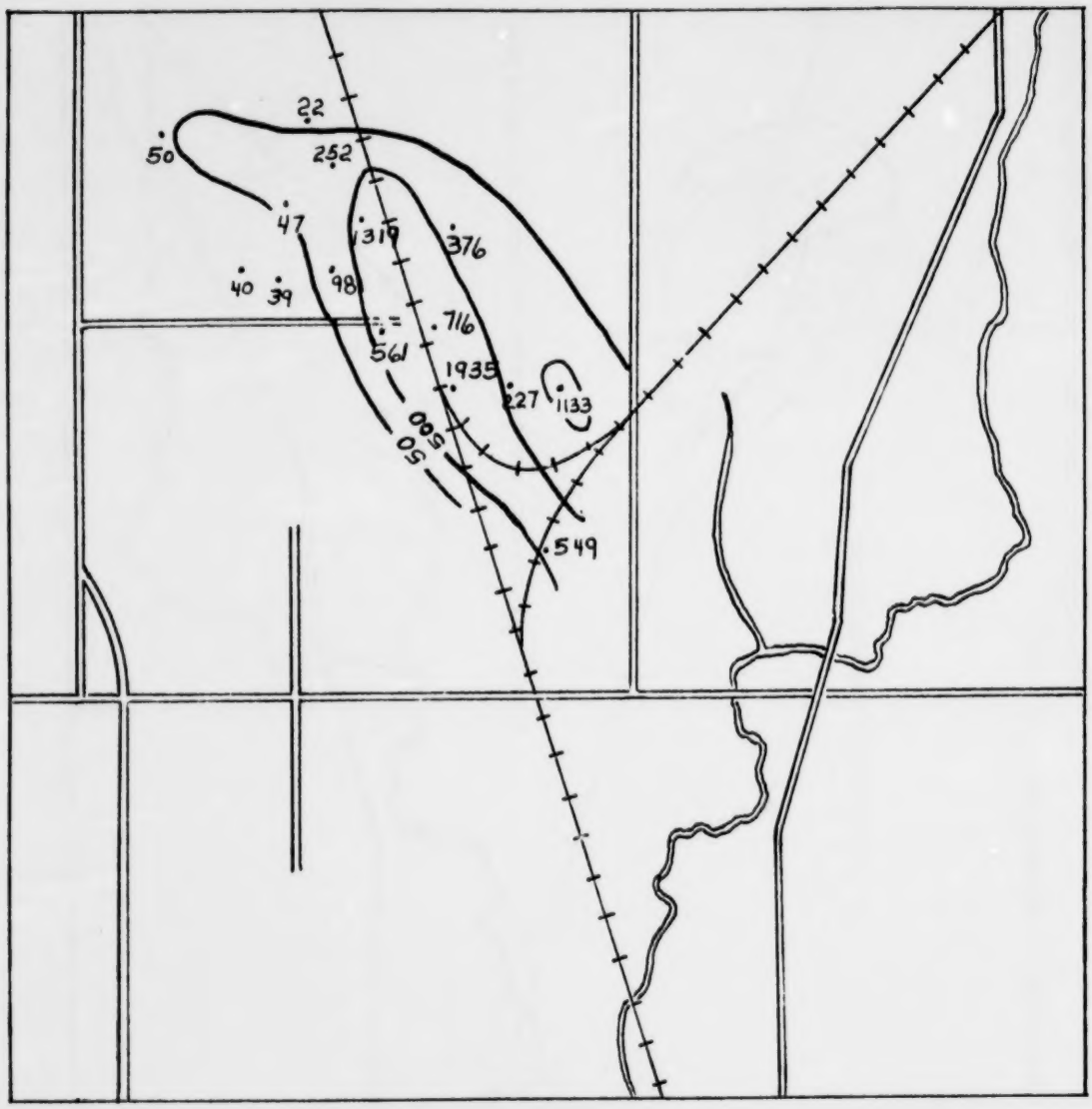


Figure 4. 1974 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from Keck (4).

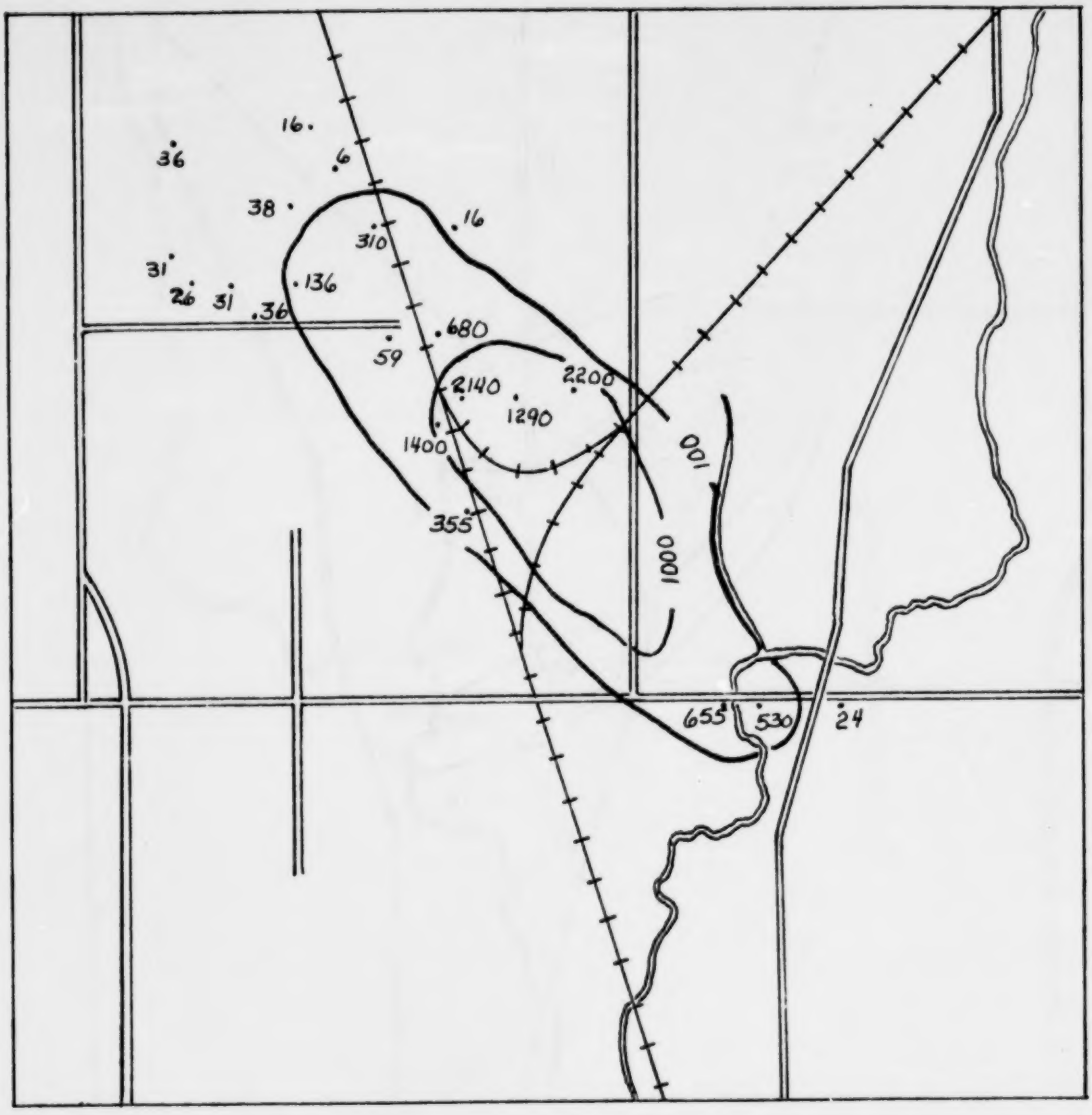


Figure 5. 1977 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from Keck (4).

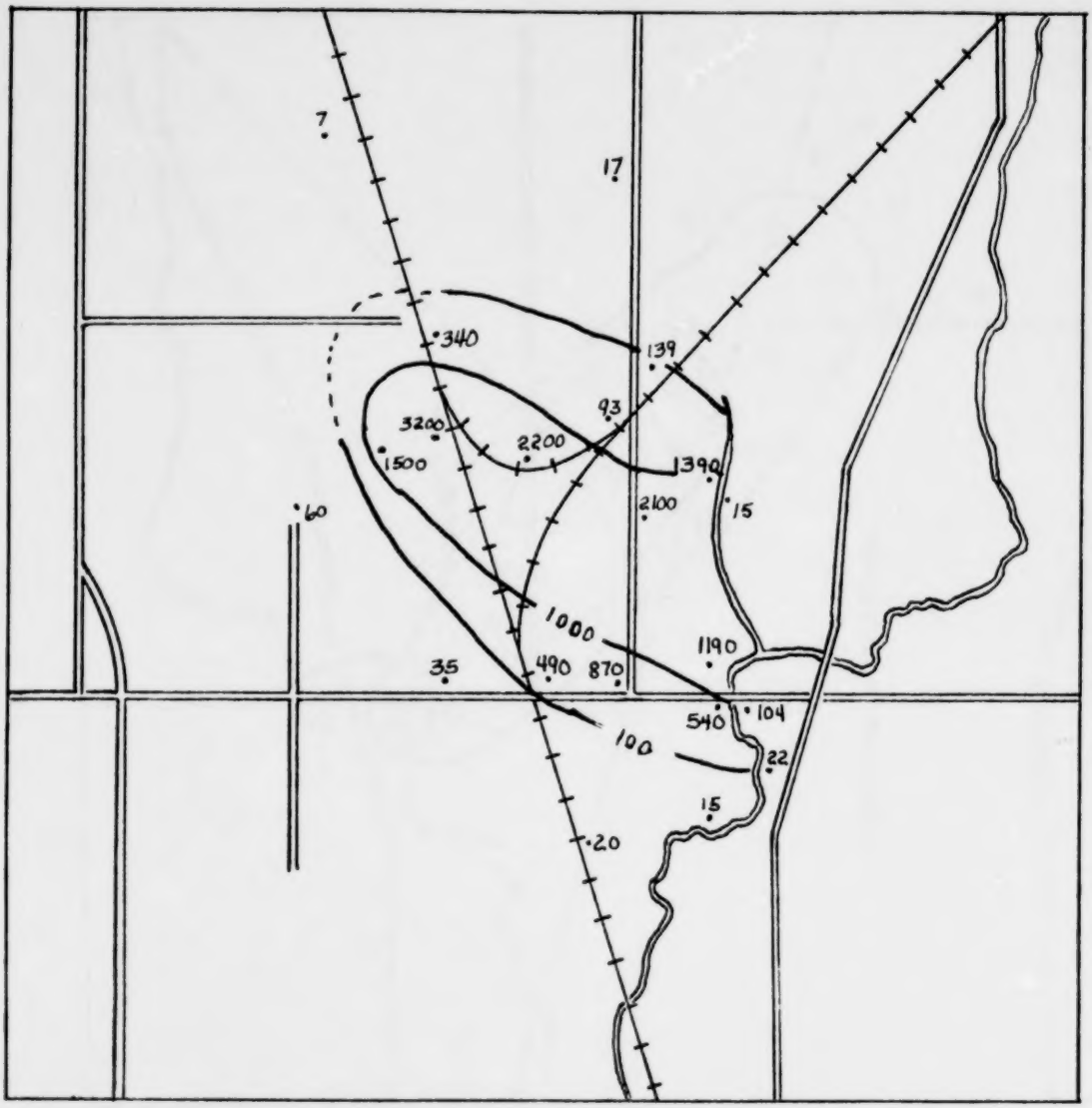


Figure 6. 1978-79 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/ℓ) from DNR (6,7).

Figure 7. 1975 Phenol Concentrations (mg/ℓ) in Deep Observation Wells (from Williams and Works (2)).

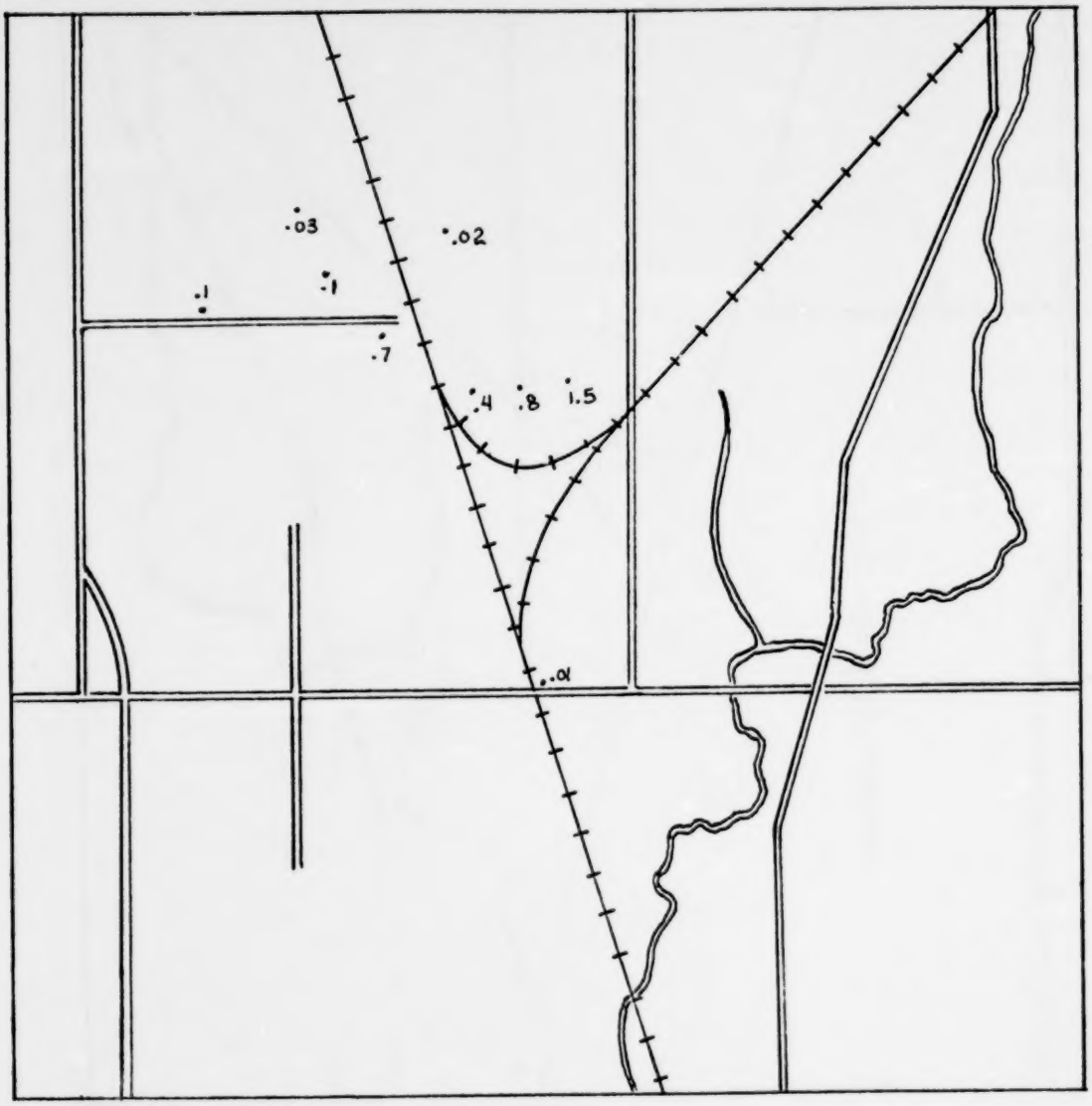


Figure 8. 1977 Phenol Concentrations (mg/ℓ) in Deep Observation Wells (from Muskegon County Health Department (5)).

Figure 9. 1978-79 Phenol Concentrations (mg/ℓ) in Deep Observation Wells (from DNR (6,7)).

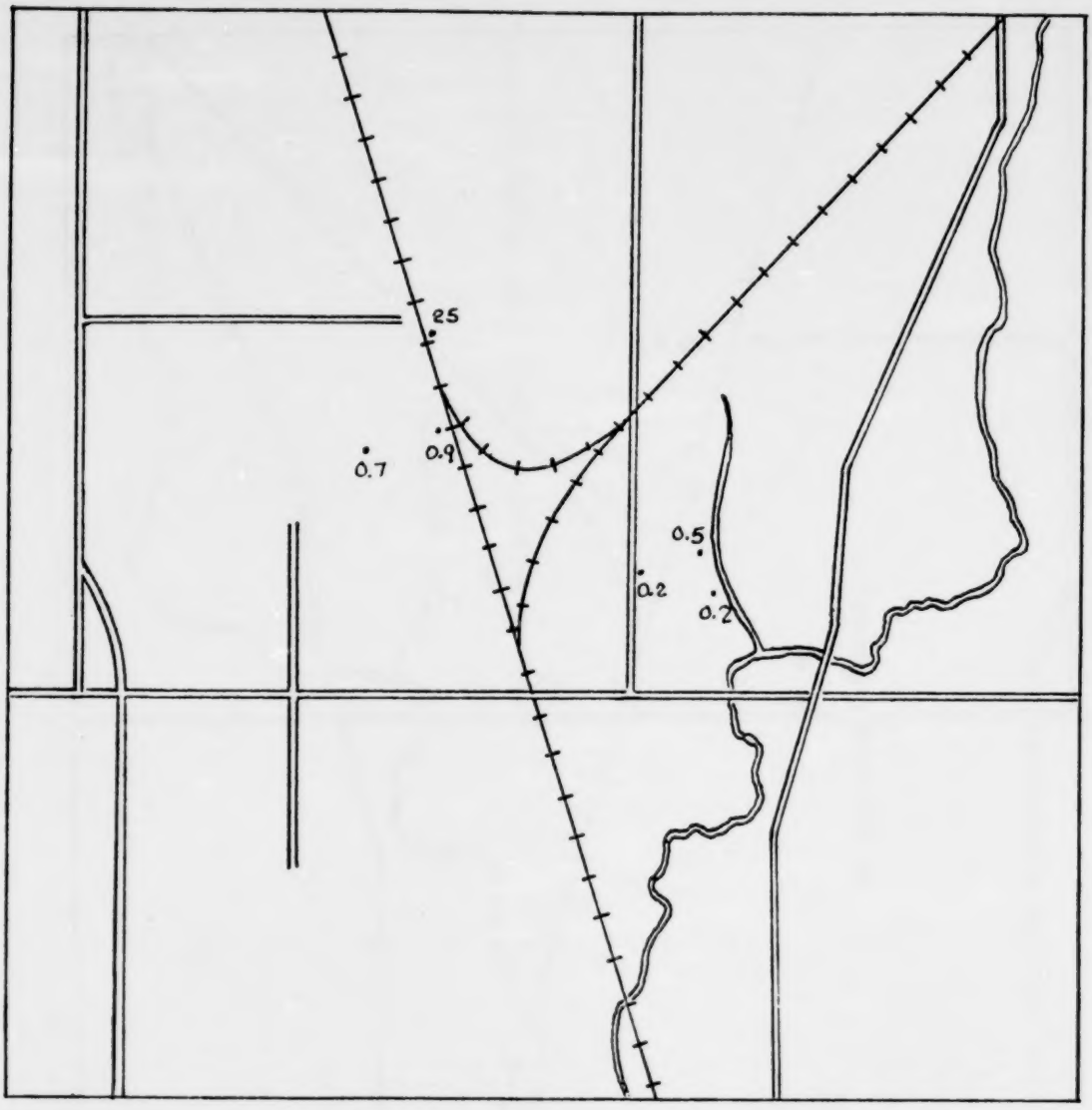


Figure 10. 1978-79 Benzene Concentrations (mg/ℓ) in Deep Observation Wells from DNP (6,7).

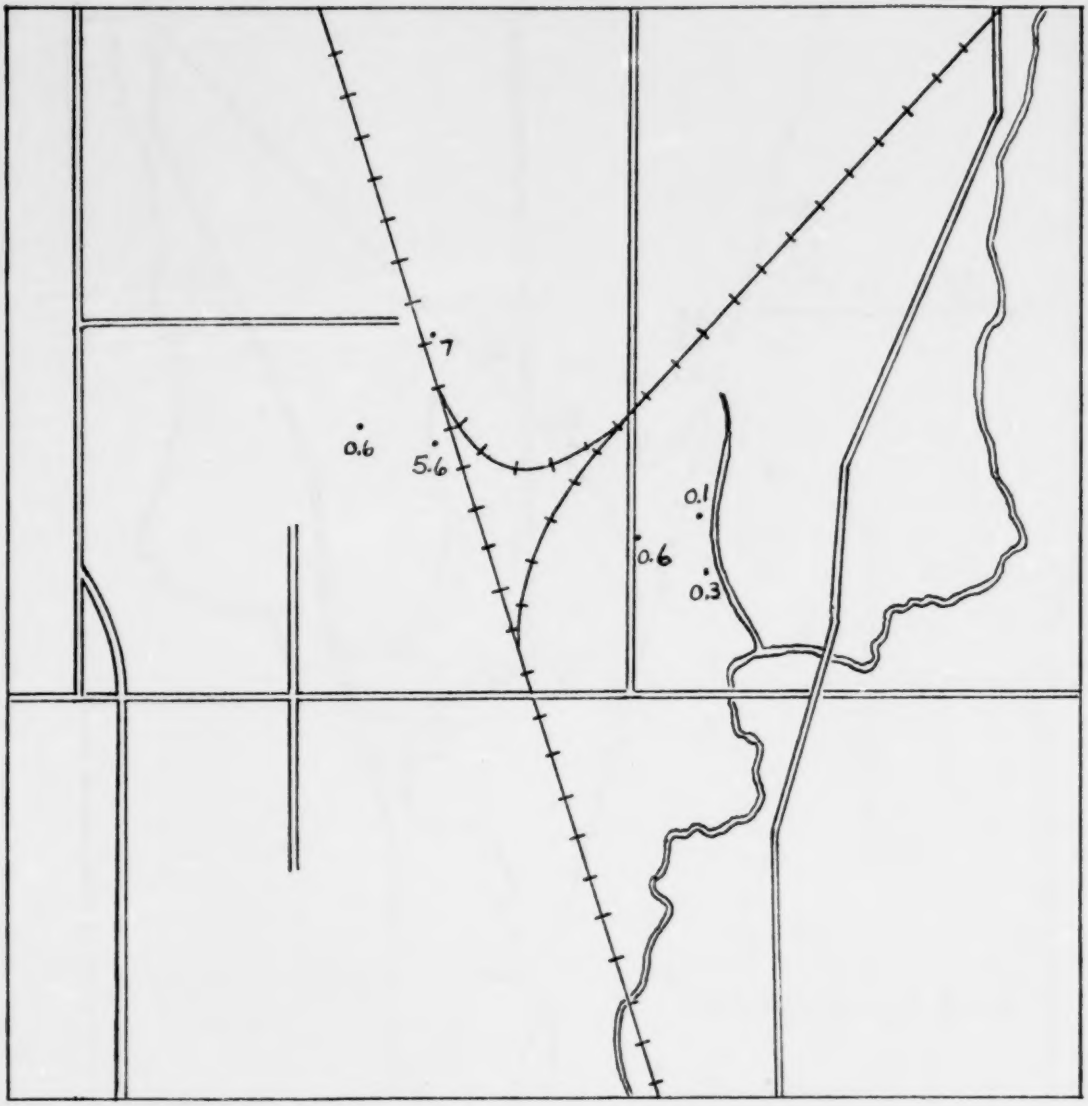


Figure 11. 1978-79 Toluene Concentrations (mg/ℓ) in Deep Observation Wells From DNR (6,7).

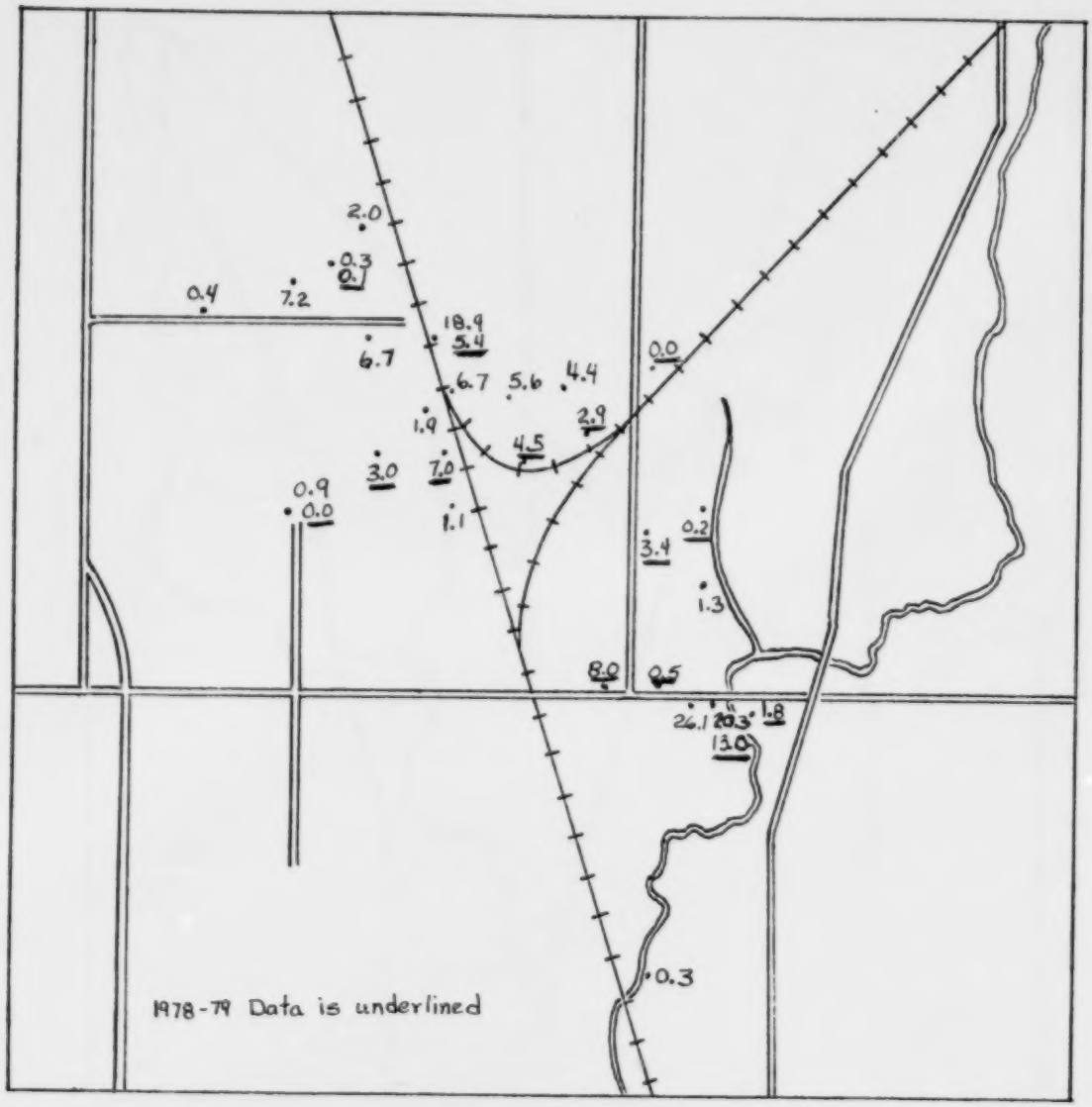


Figure 12. 1977-79 Aromatic Amines Concentrations (mg/ℓ) in Deep Observation Wells from DNR (6,7).

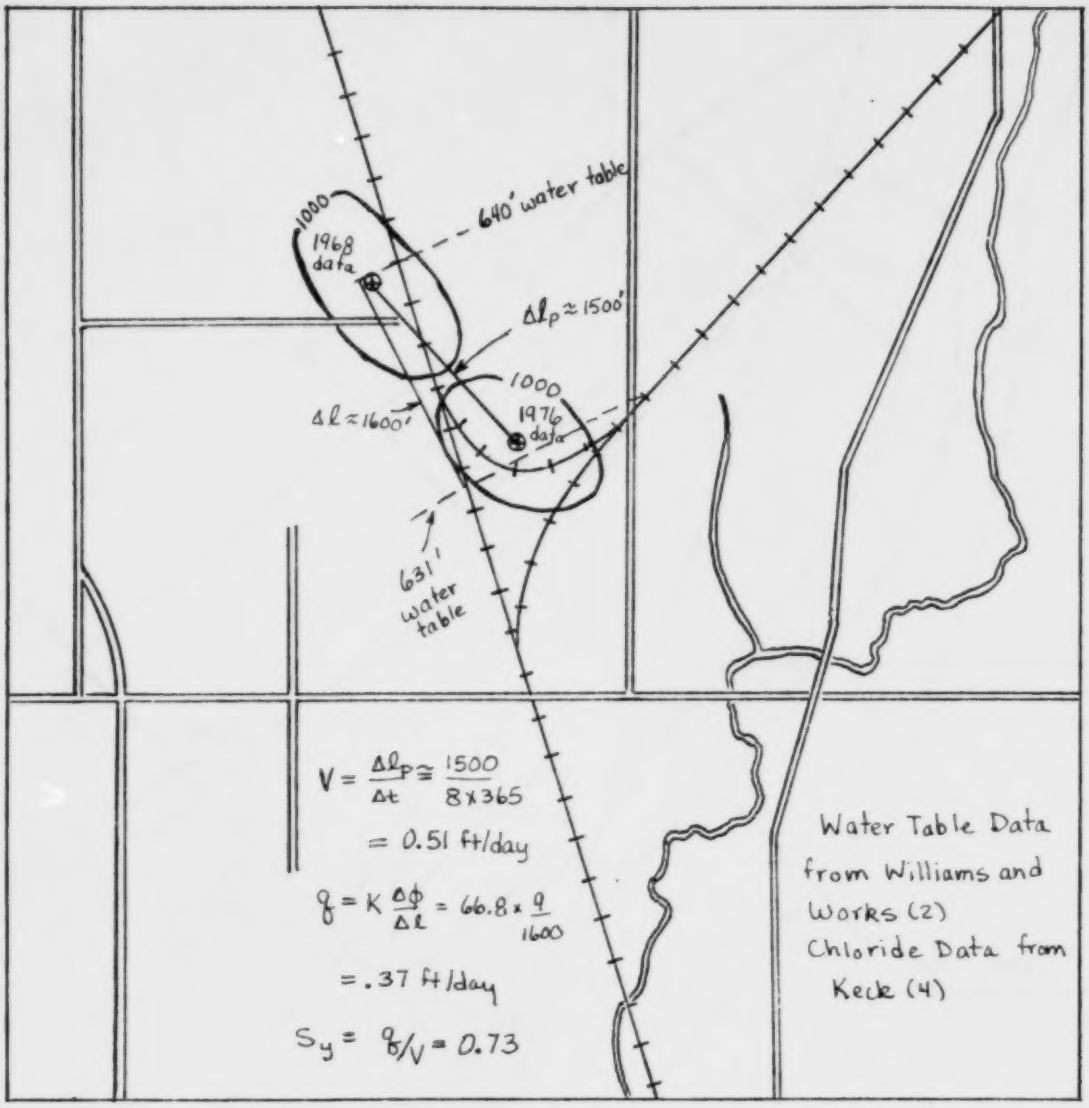

1000
1968 data
640' water table
$\Delta l_p \approx 1500'$
1000
1976 data
$\Delta l \approx 1600'$
631' water table
$V = \frac{\Delta l_p}{\Delta t} \approx \frac{1500}{8 \times 365}$
$= 0.51$ ft/day
$q = K \frac{\Delta \phi}{\Delta l} = 66.8 \times \frac{q}{1600}$
$= .37$ ft/day
$S_y = q/V = 0.73$
Water Table Data from Williams and Works (2)
Chloride Data from Keck (4)

Figure 13. Example Calculation of Specific Yield.

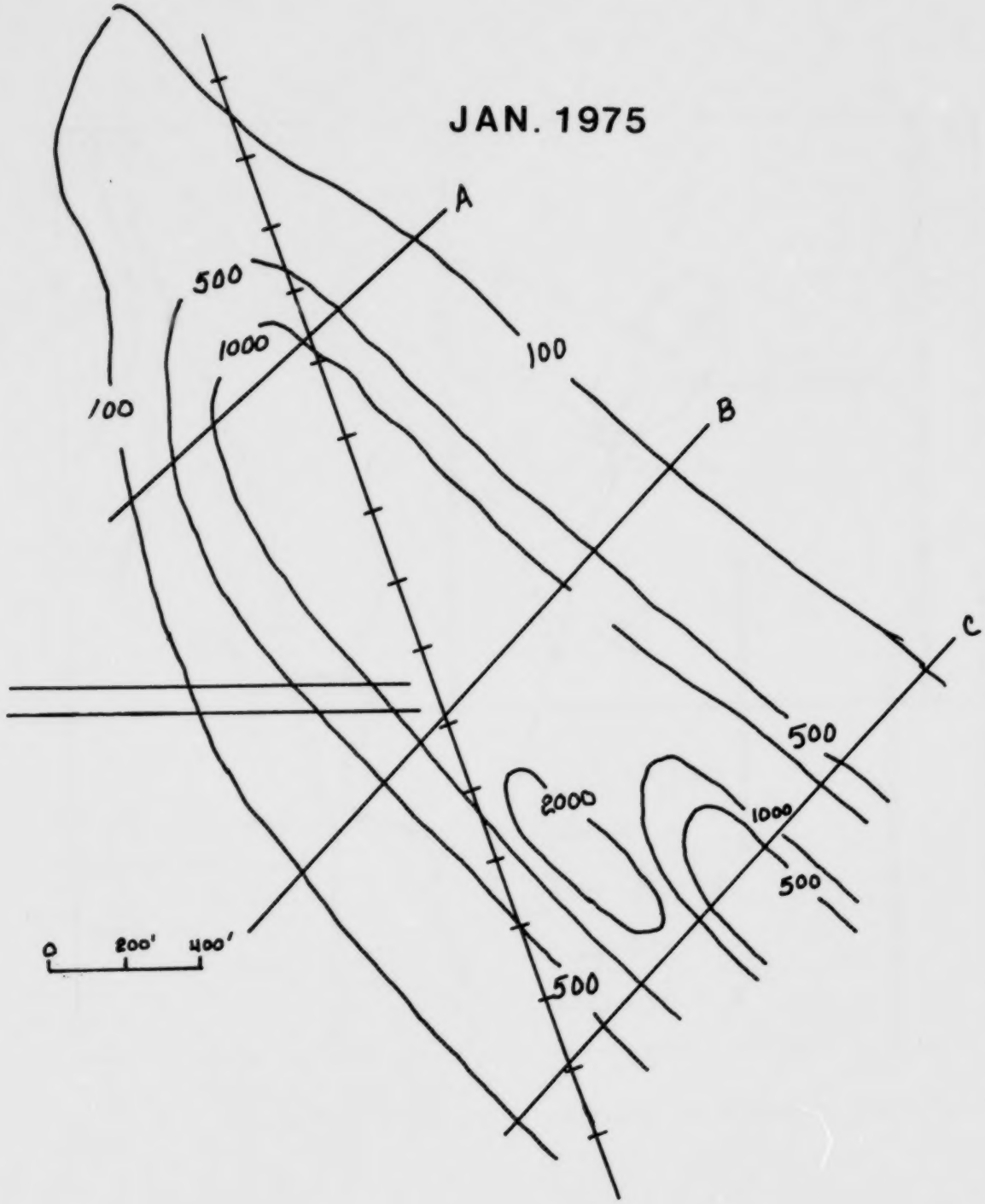


Figure 14. Chloride Plume Detail for Computation of Lateral Dispersivity (from Williams and Works (2)).

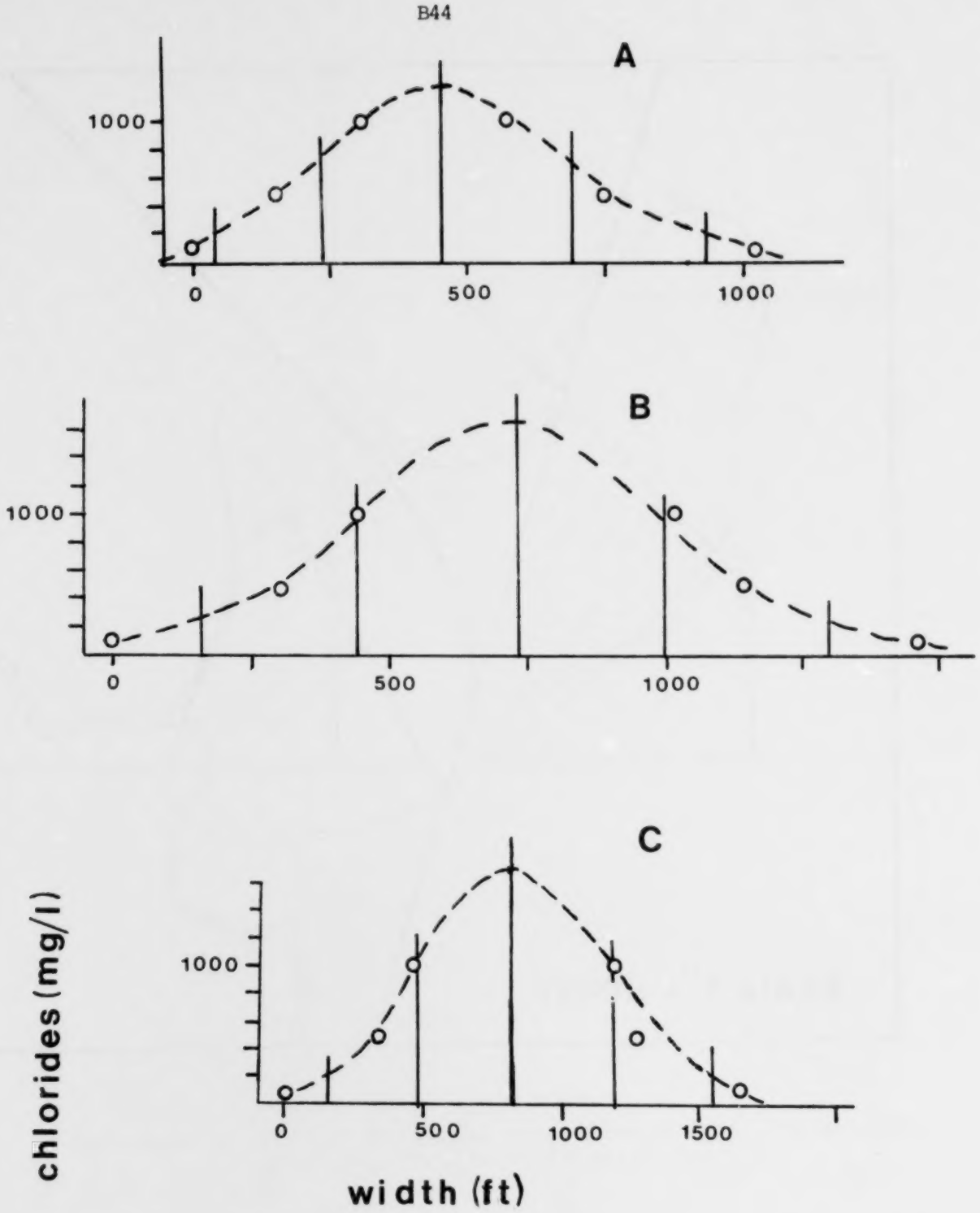


Figure 15. Cross-Sectional Concentration Profiles, Jan. 1975 (from Williams and Works (2)).

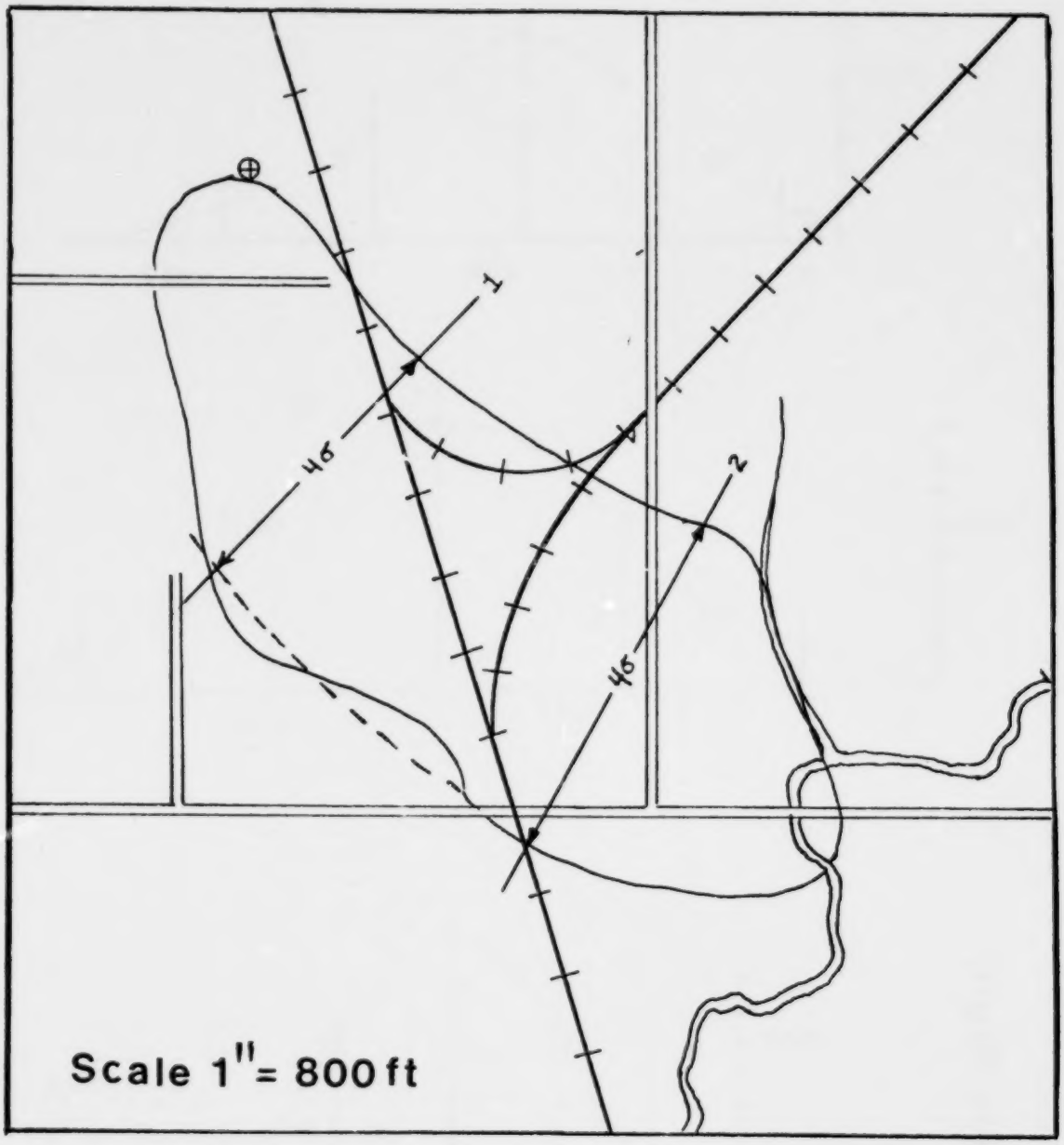


Figure 16. 1979 Plume Extent Estimated by Keck (9) used for Computation of Lateral Dispersivity.

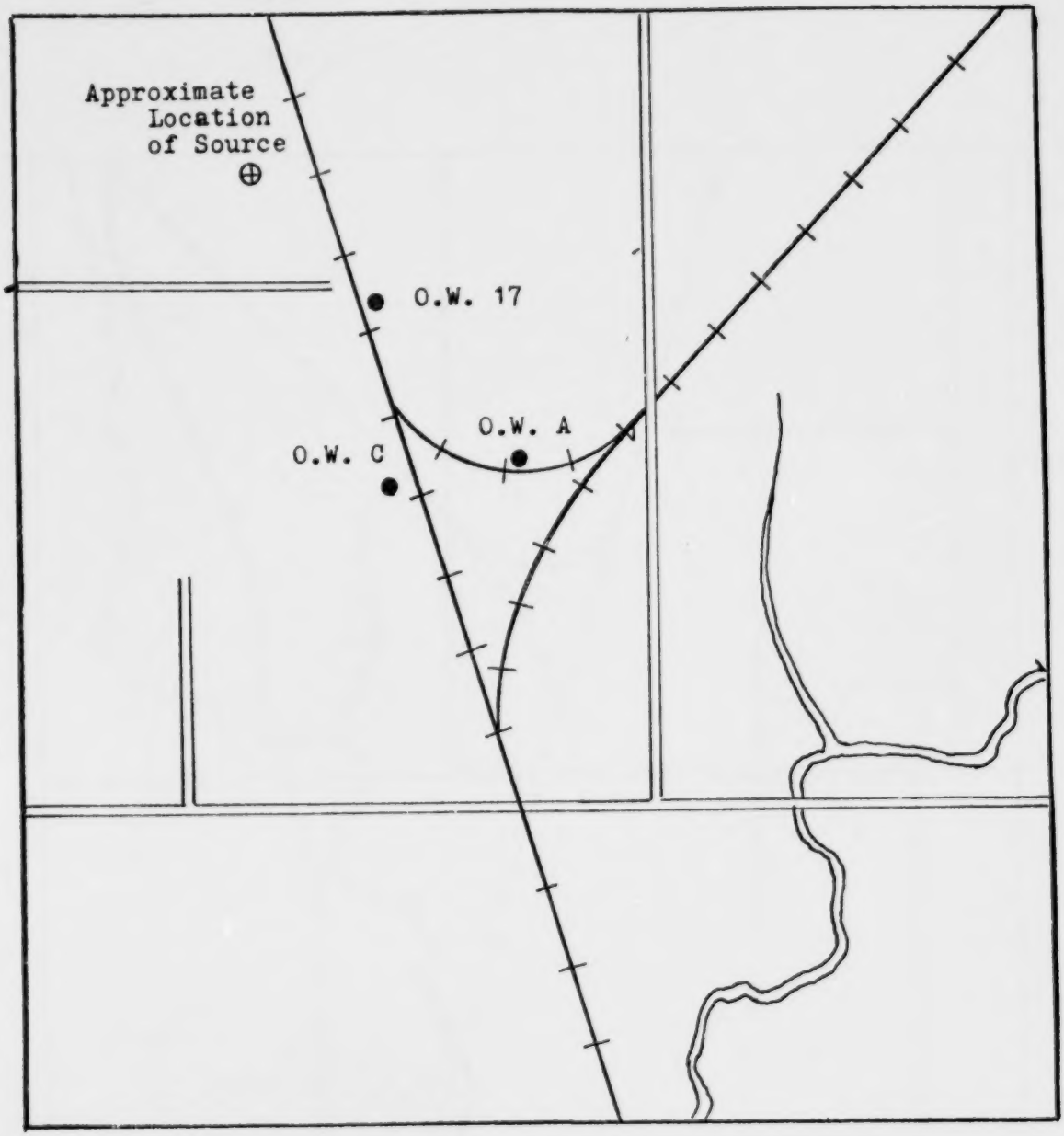


Figure 17. Source and Observation Well Locations.

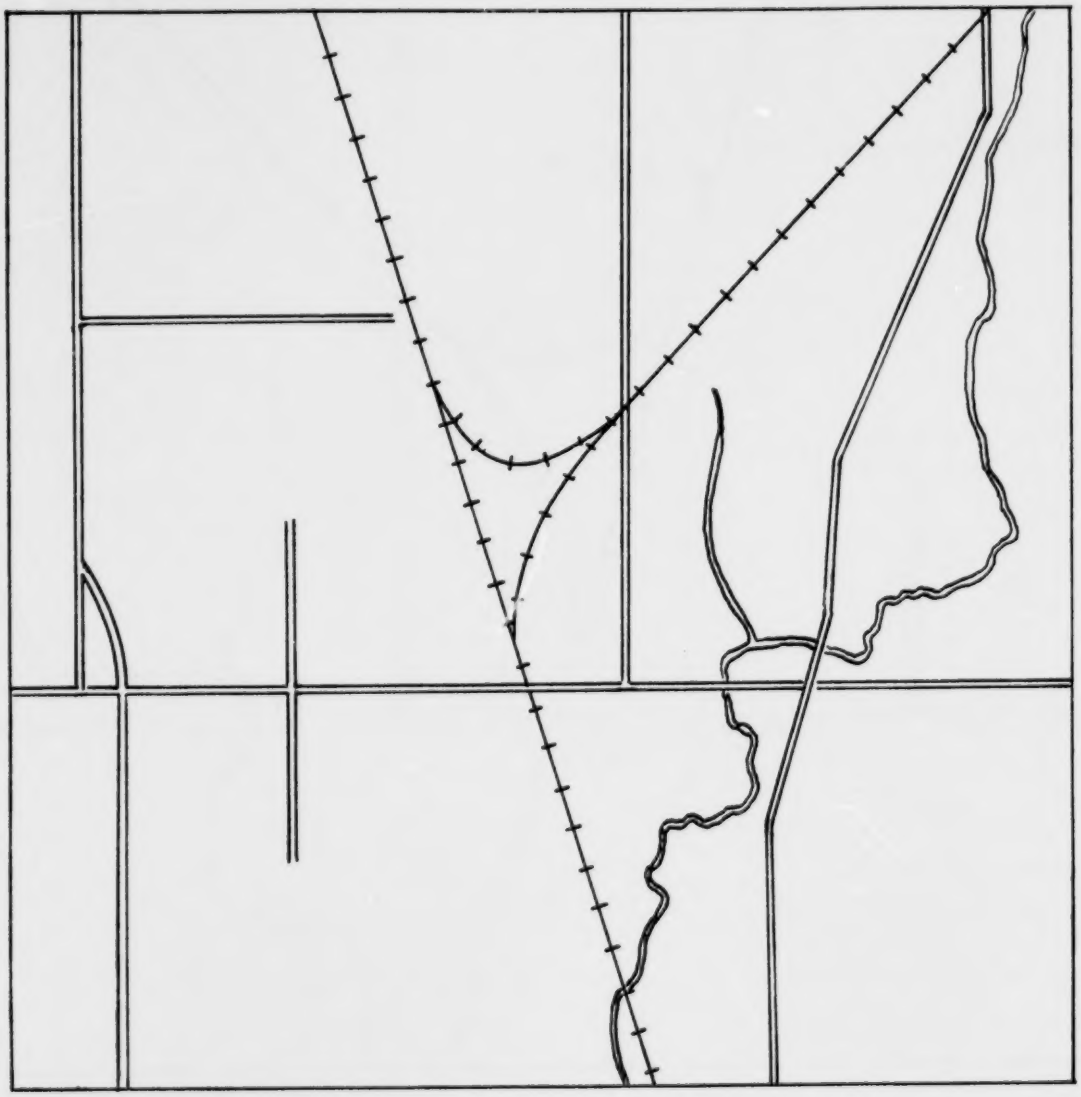
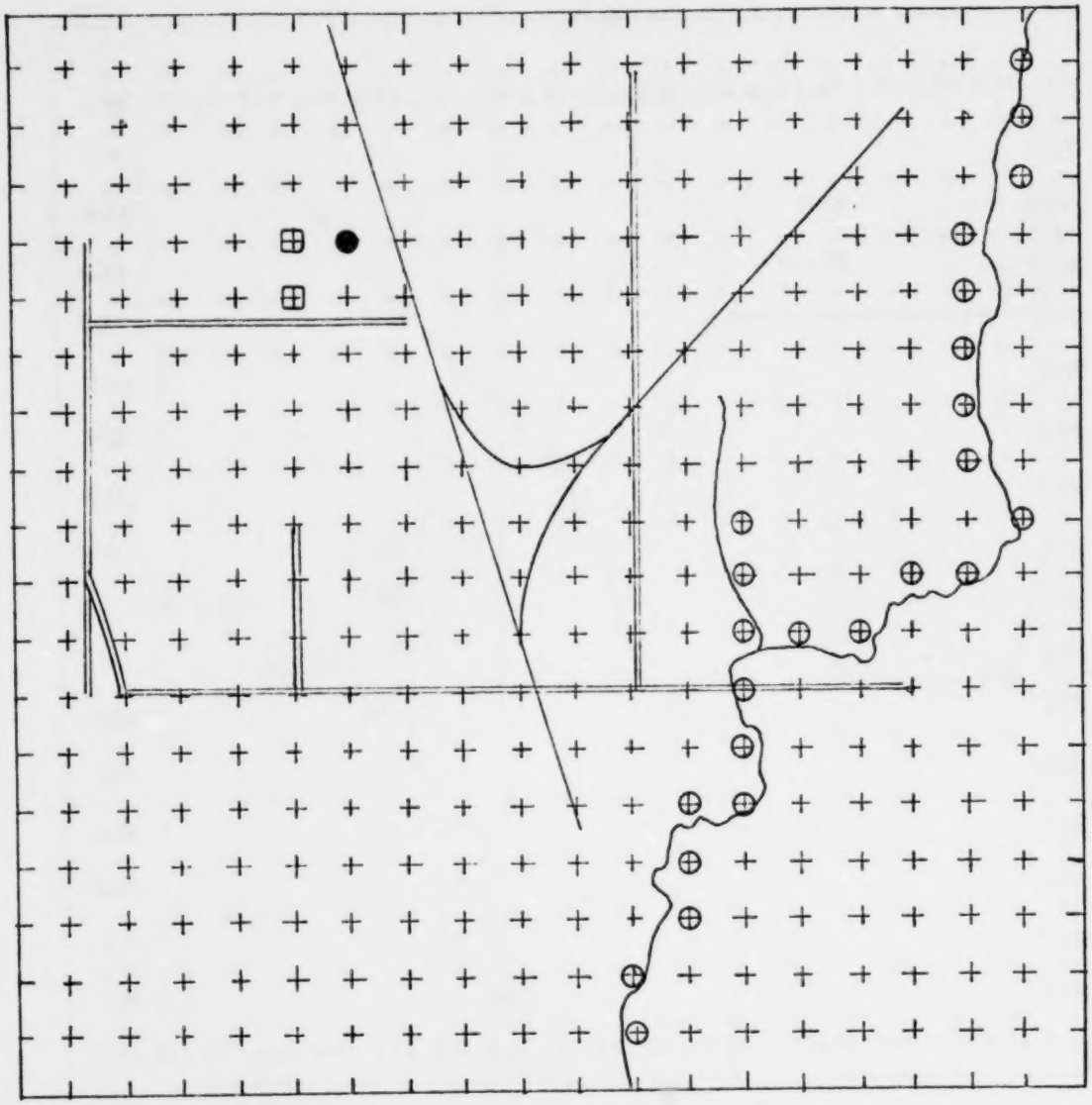


Figure 18. Area Covered by Numerical Model.



⊞ Pumping Nodes with Specified Heads

⊕ Creek Nodes with Specified Heads

● Contaminant Source Node

Figure 19. Grid Detail for Numerical Model.

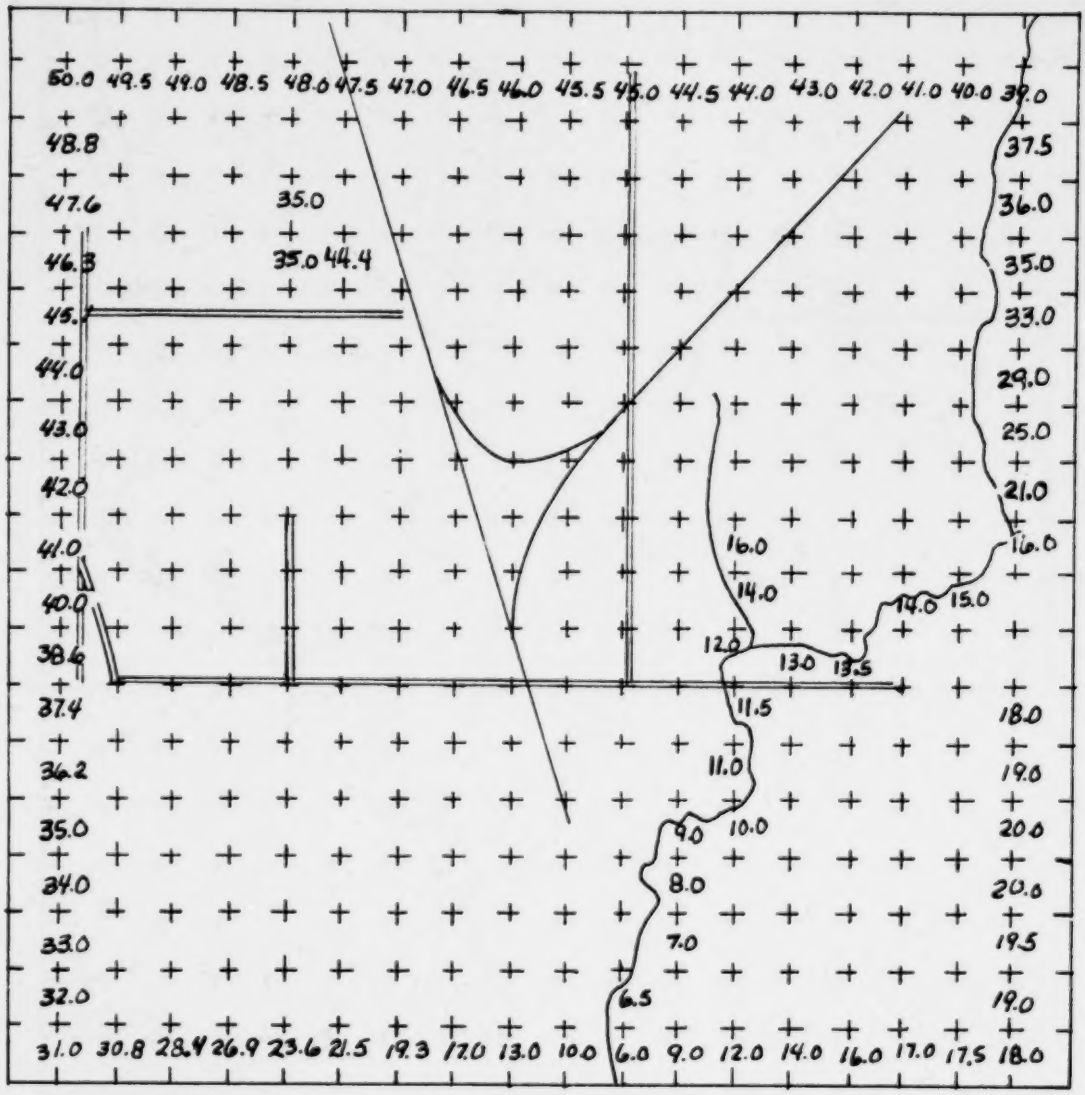


Figure 20. Specified Heads used in Final Numerical Simulation.

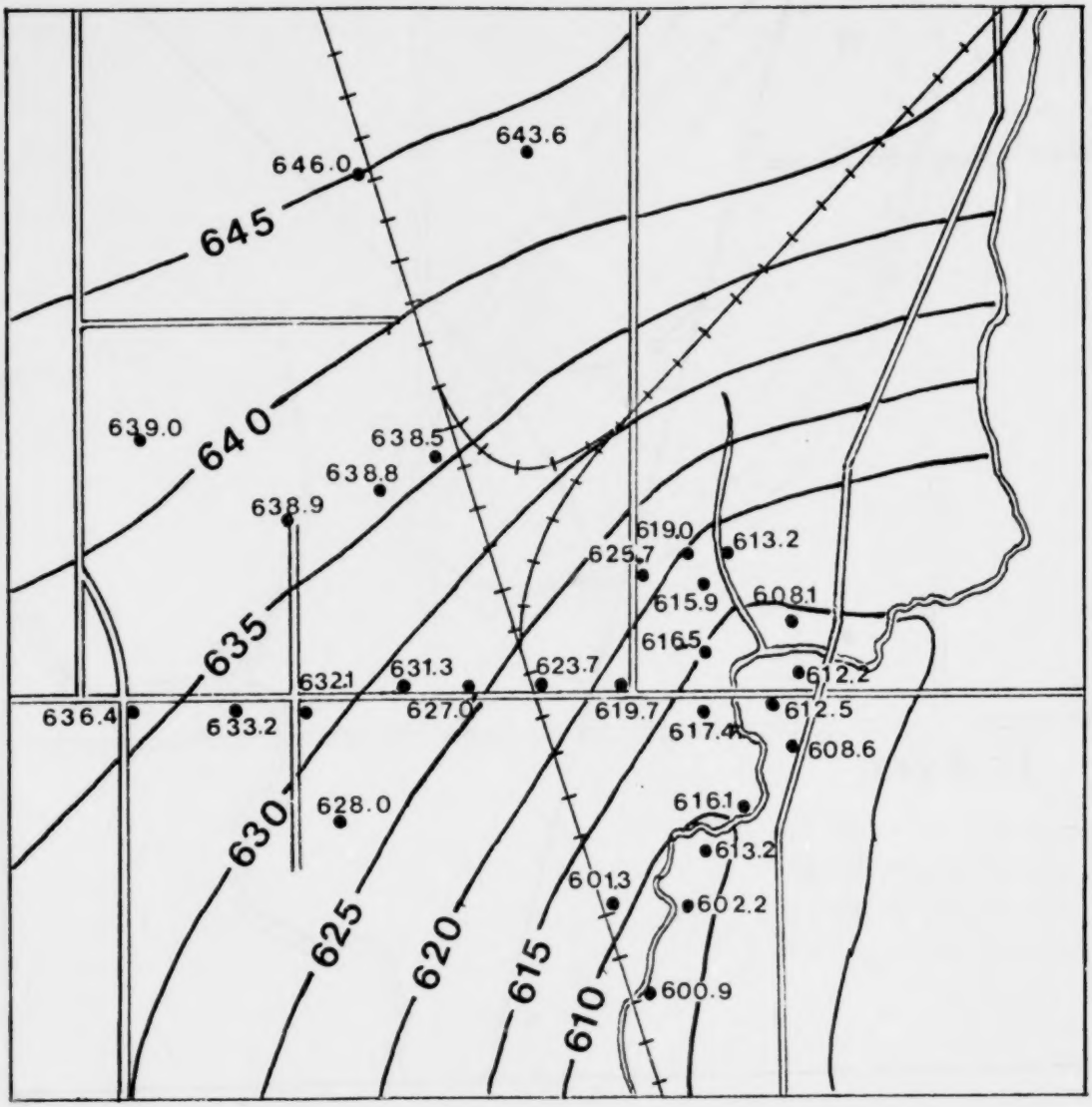


Figure 21. Final Water Table Simulation and Comparison of Water Table Data from Keck (8).

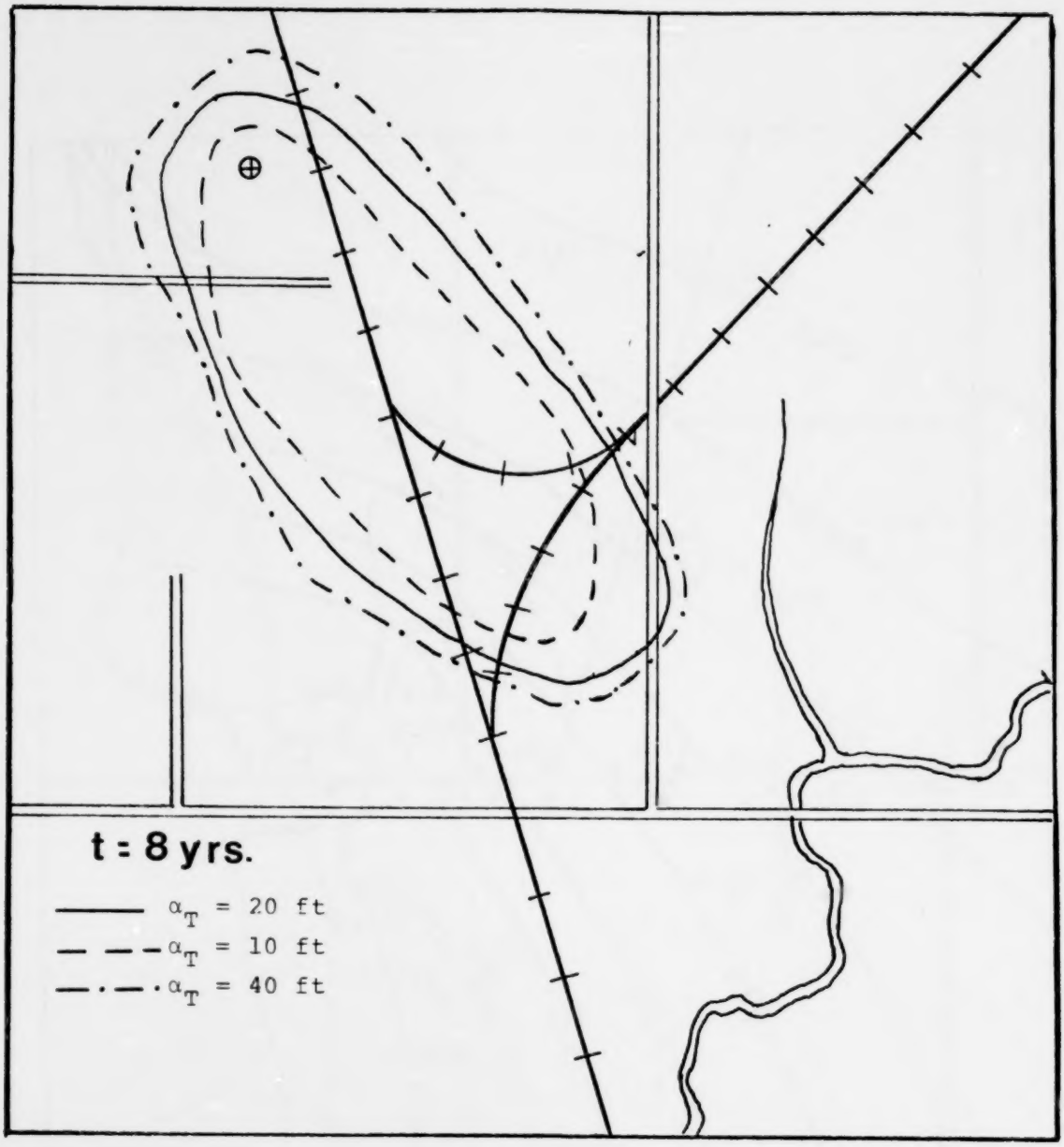


Figure 22. Sensitivity of Plume Extent to Variations in α_T.

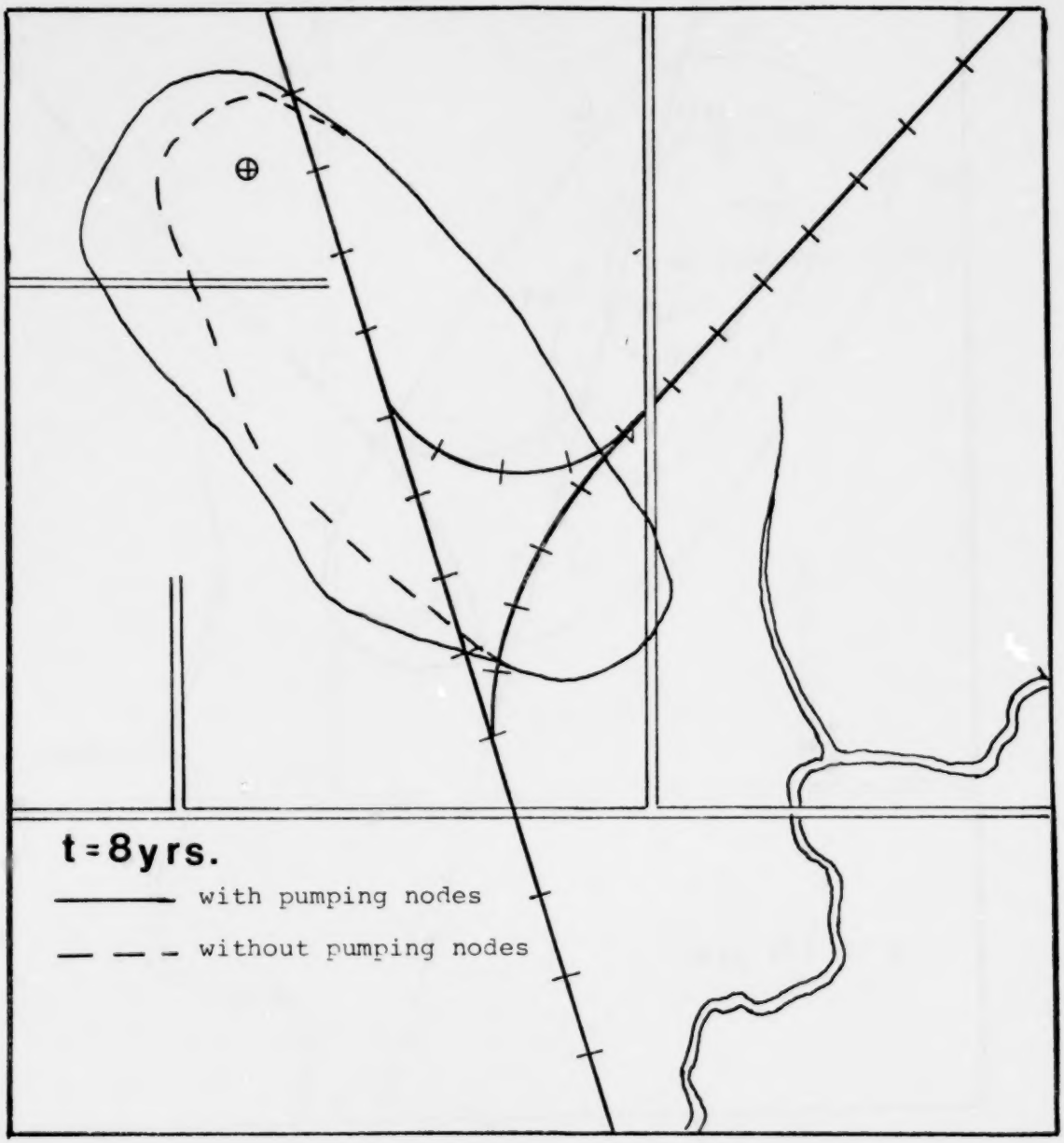


Figure 23. Comparison of Effect of Pumping Nodes on Chloride Plume Extent.

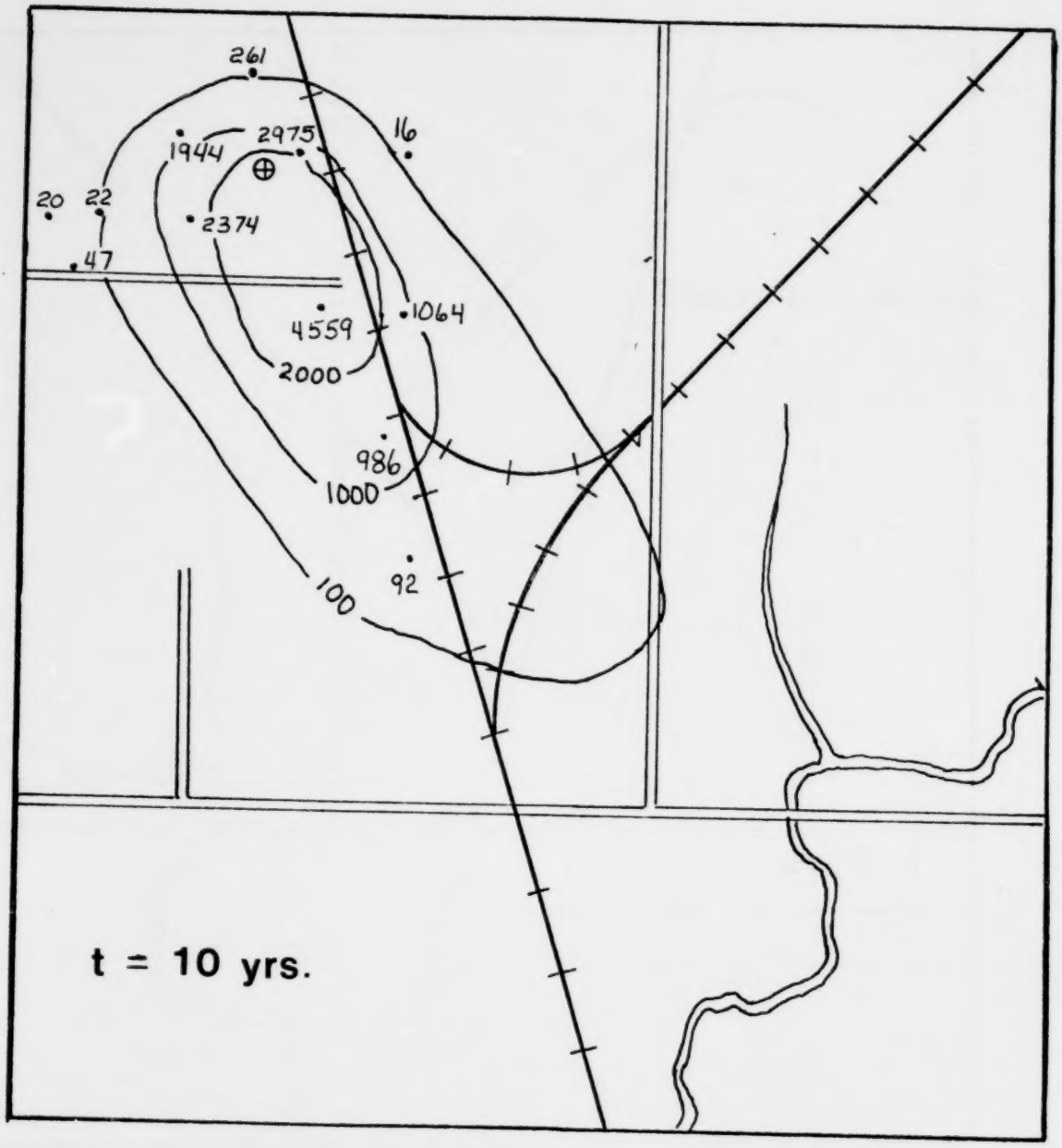


Figure 24. Comparison of 10 Year Numerical Simulation with 1968 Chloride Data (concentration mg/ℓ).

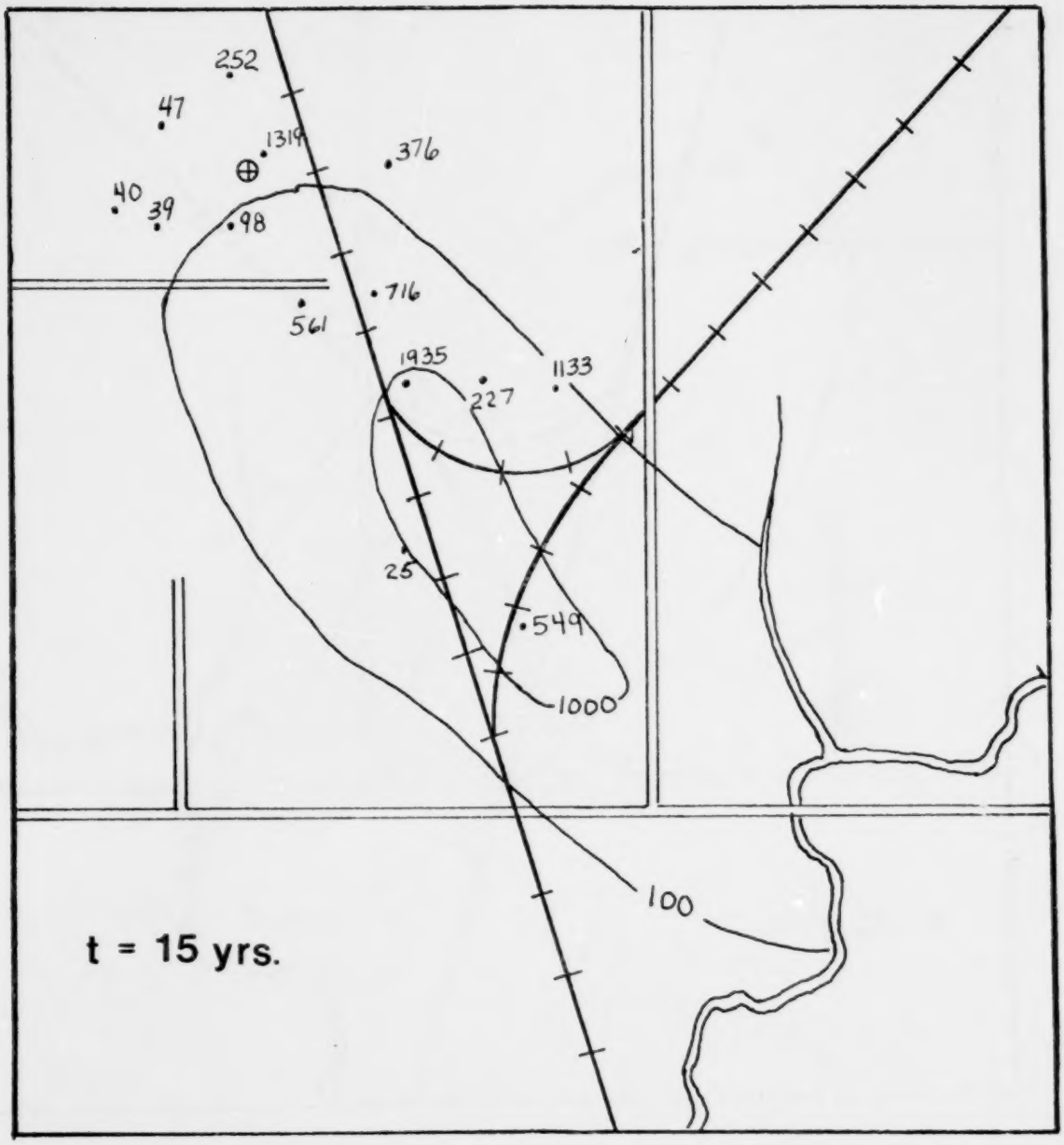


Figure 25. Comparison of 15 Year Numerical Simulation with 1974 Chloride Data (concentration in mg/ℓ).

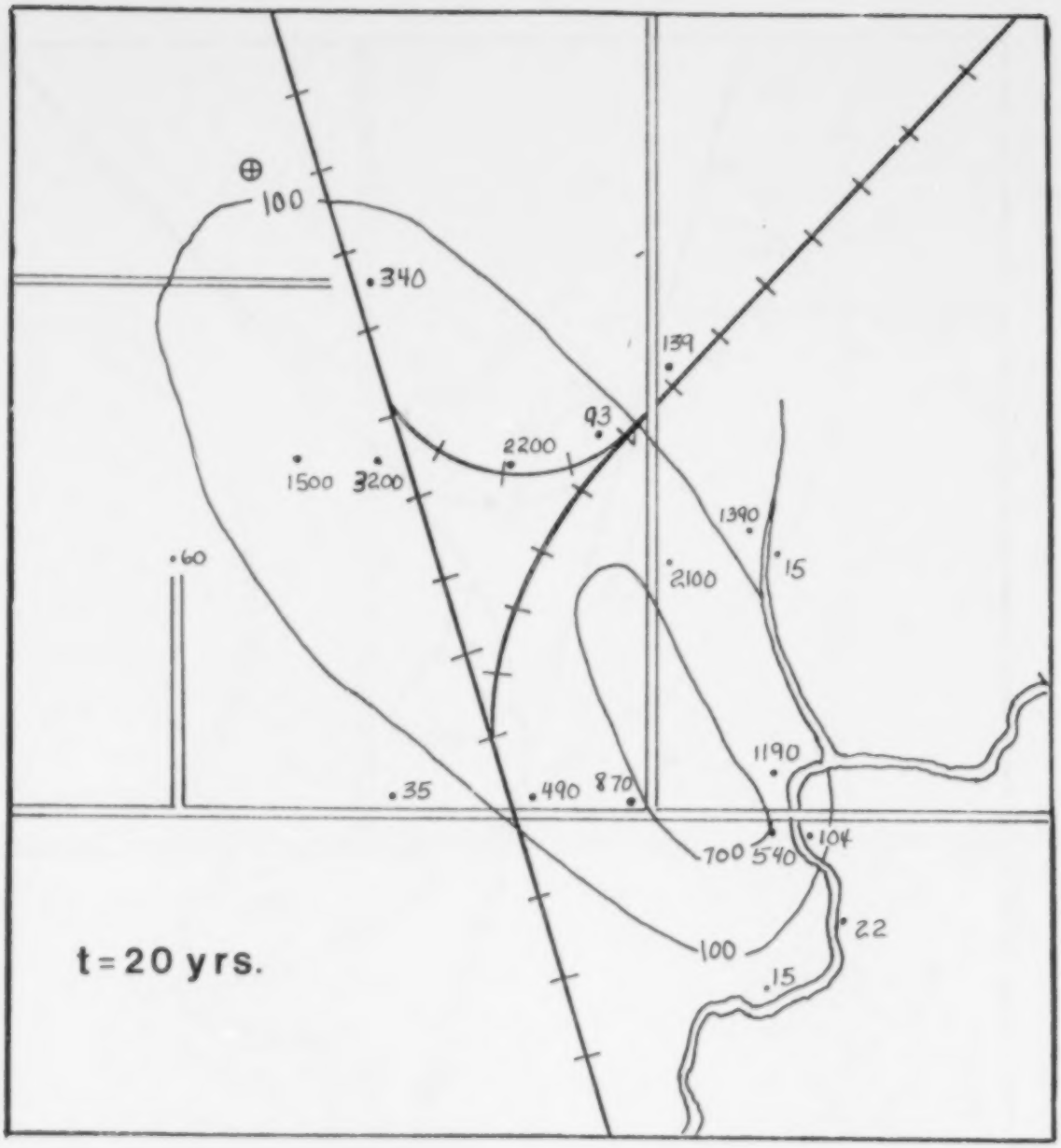


Figure 26. Comparison of 20 Year Numerical Simulation with 1978-79 Chloride Data (concentration in mg/ℓ).

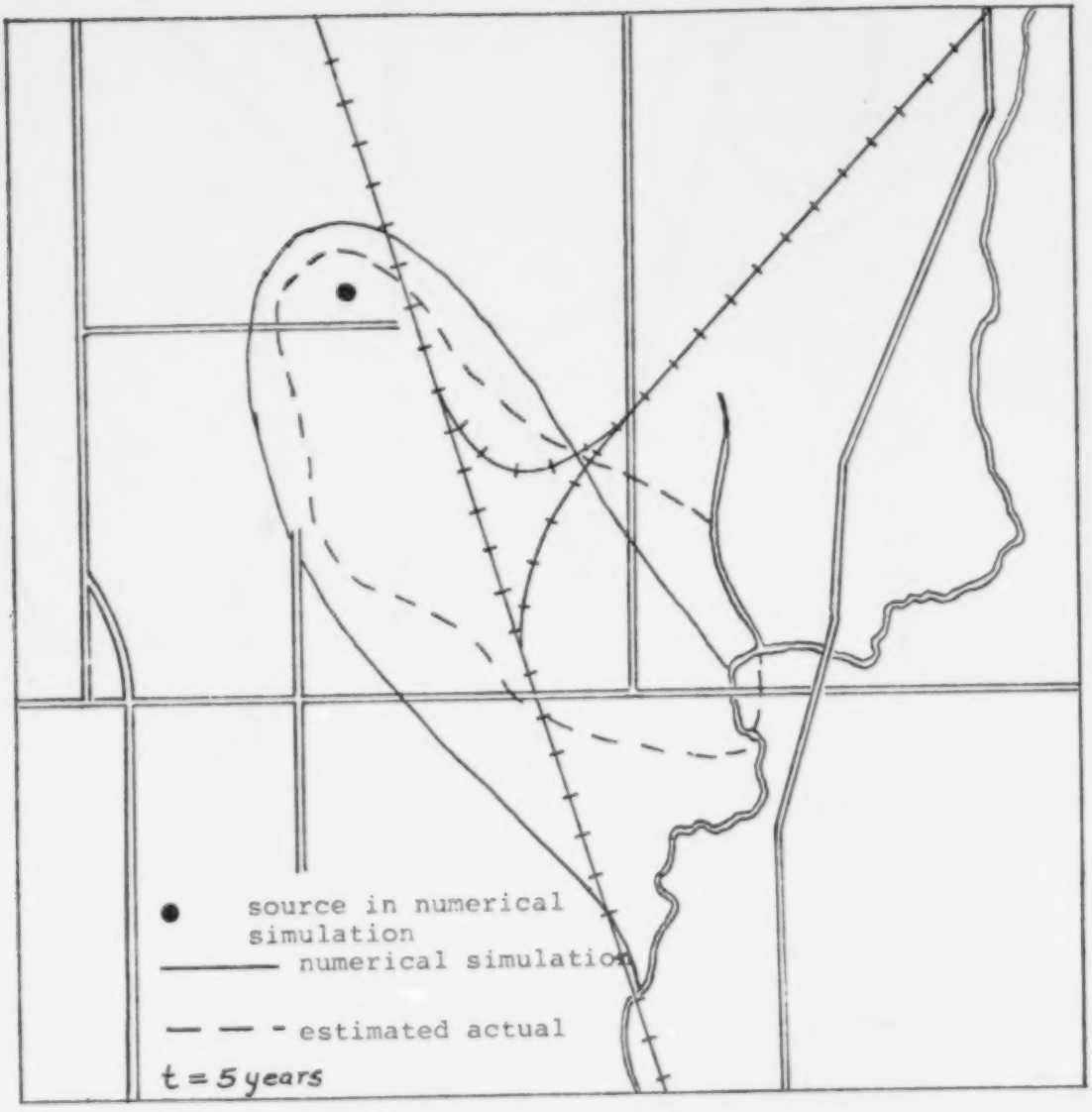


Figure 27. Comparison of Simulated Plume Extent with Aquifer Parameters Estimated by Keck (8) and Chloride Plume in 1978-79.

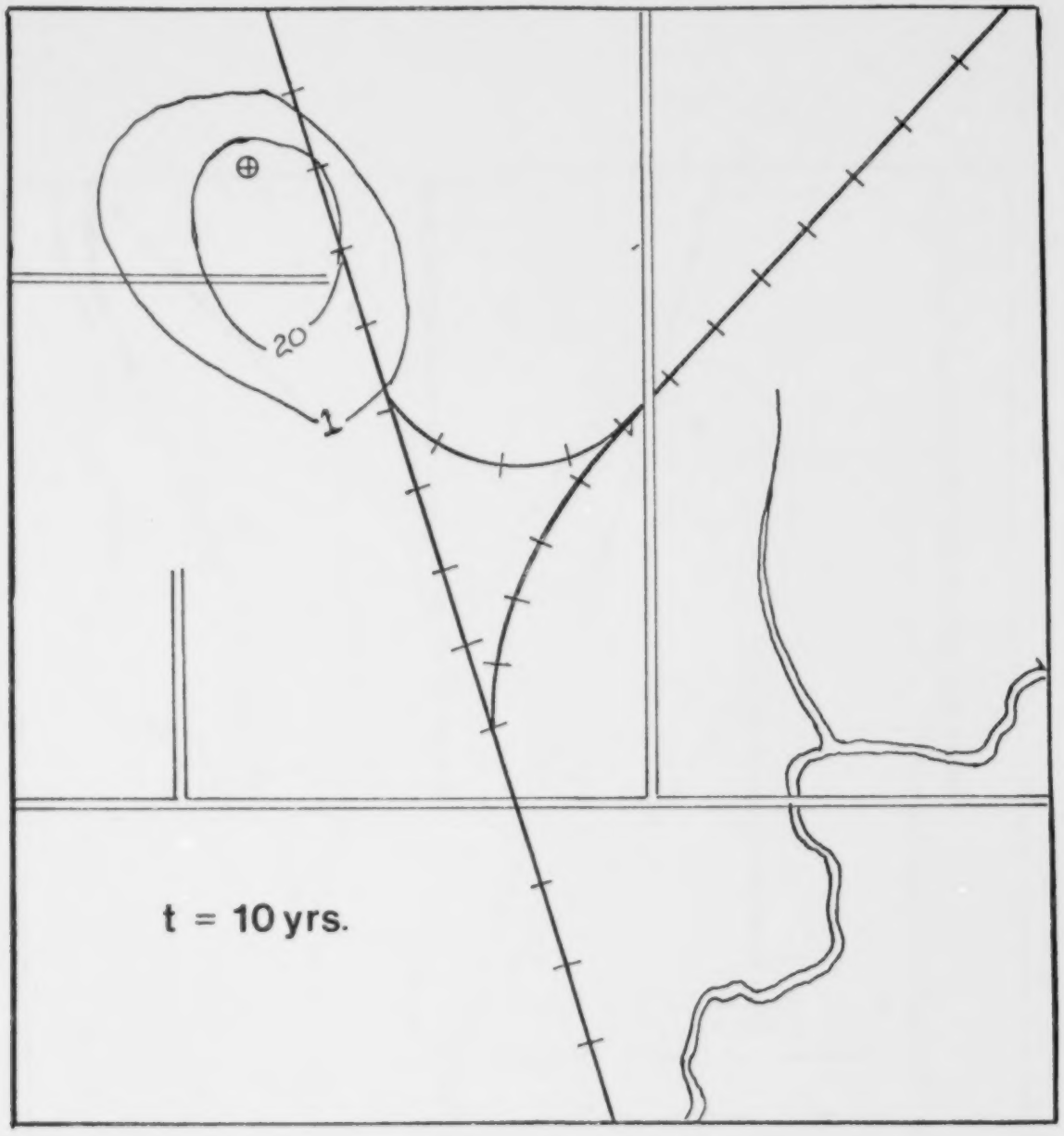


Figure 28. Concentration (mg/ℓ) profile for Phenol after 10 Years. Retardation Factor of 3.

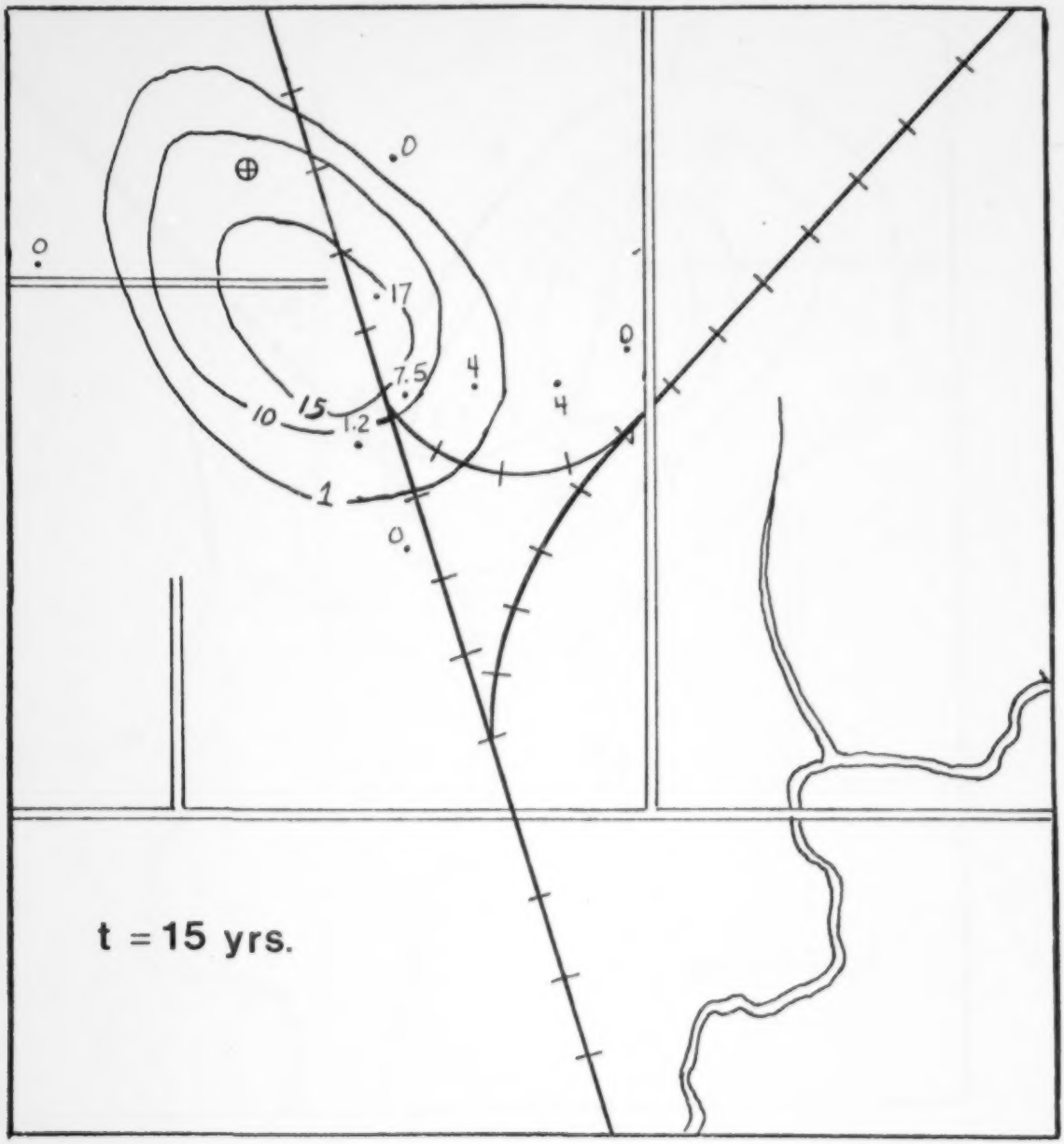


Figure 29. Comparison of 15 Year Numerical Simulation with 1975 Phenol Concentrations (mg/ℓ) Retardation Factor of 3.

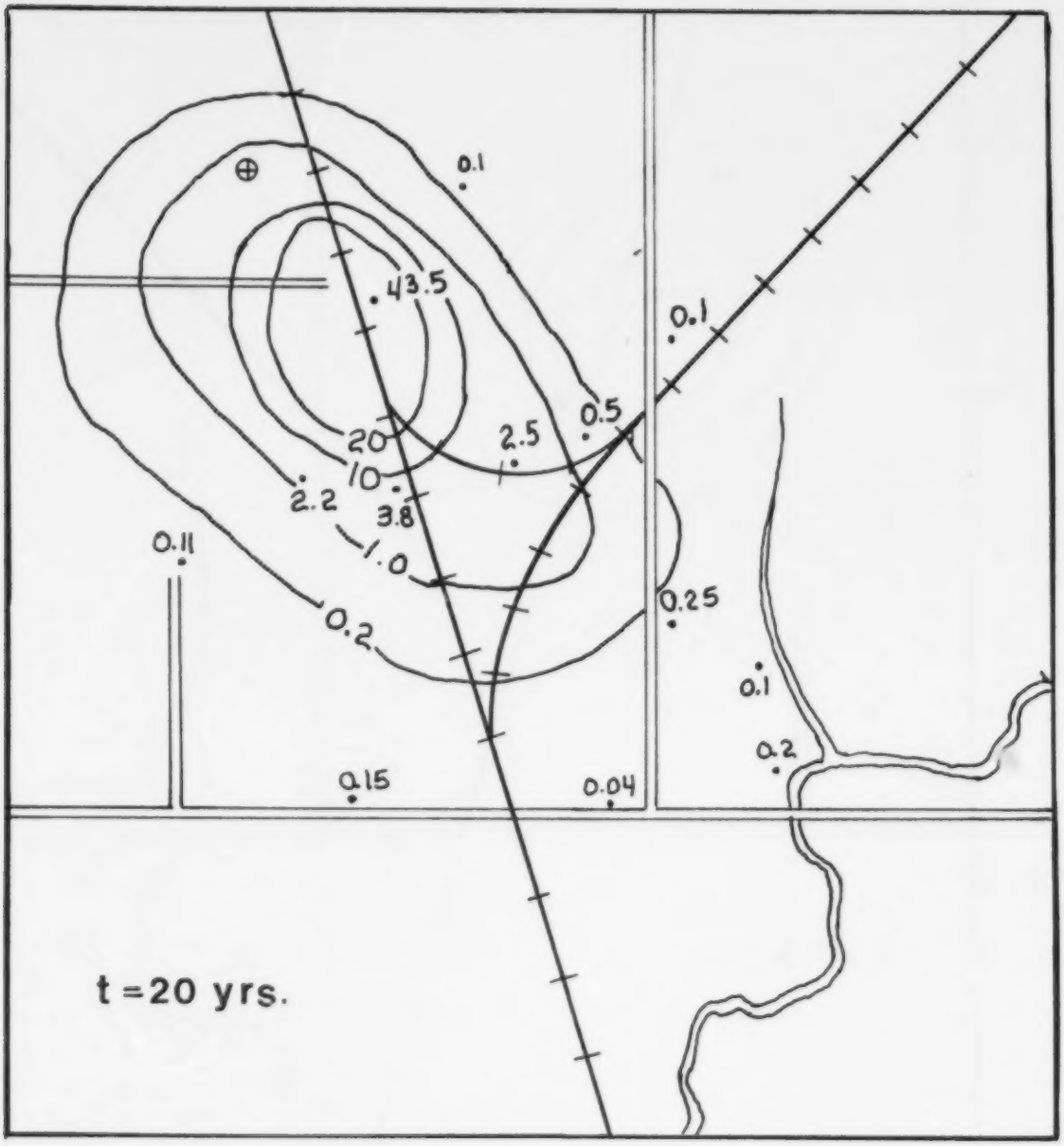


Figure 30. Comparison of 20 Year Numerical Simulation with 1978-79 Phenol Concentrations (mg/ℓ). Retardation Factor 3.

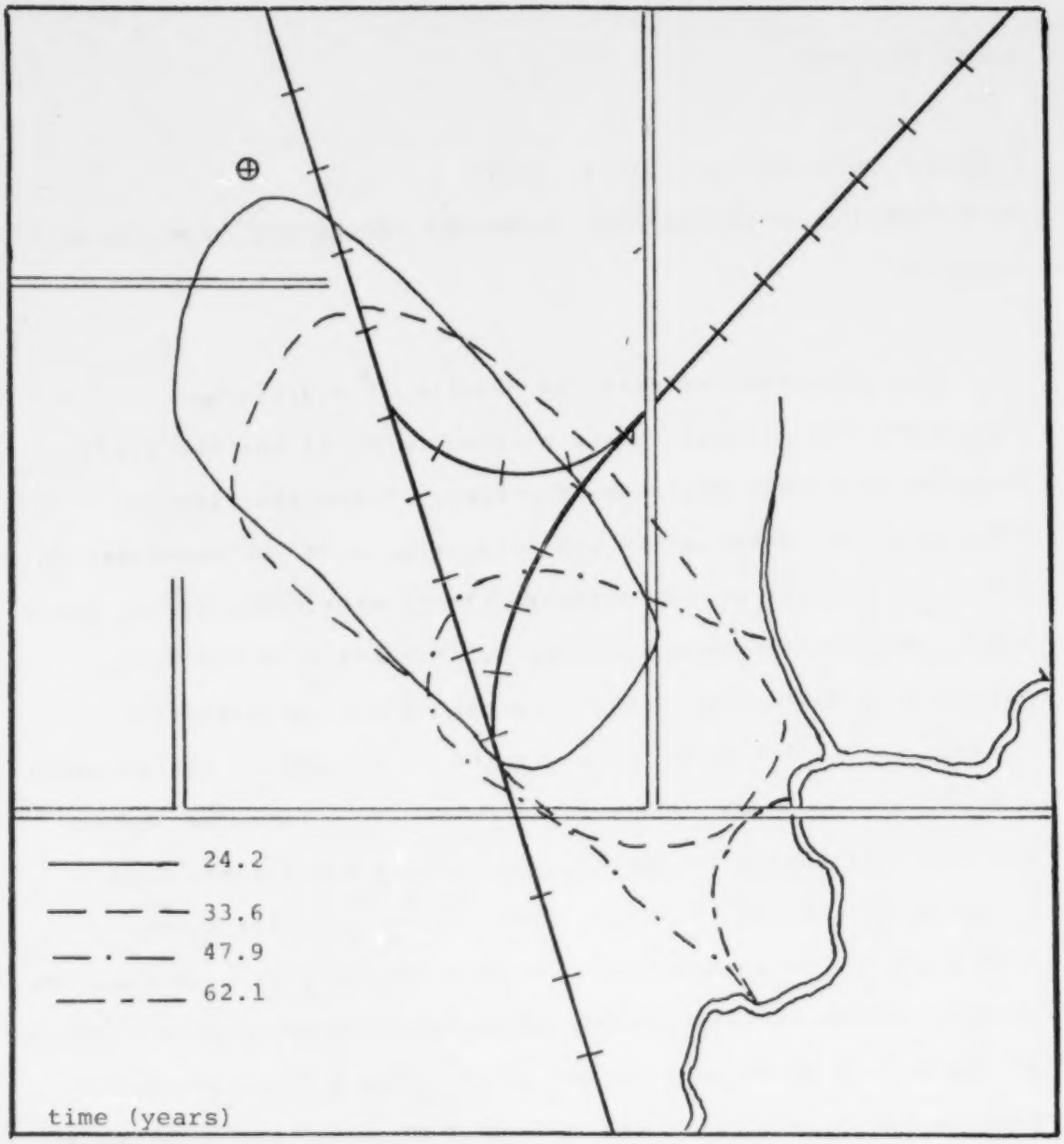


Figure 31. Development of Simulated Phenol Plume with Time.

March 20, 1982

ADDENDUM TO REPORT OF July 1, 1981:
INVESTIGATION OF CONTAMINANT TRANSPORT PARAMETERS IN MICHIGAN AQUIFERS

This addendum contains the results of additional investigations related to the original work at the Ott-Story Chemical site near Muskegon, Michigan. These additional considerations arose after the discussion with DNR personnel in which the results of the original report were presented in July, 1981. Additional questions arose with respect to the phenol simulations discussed in the original report, specifically related to (1) The sensitivity to the values of the longitudinal dispersivity and (2) Magnitudes of previously reported values for the retardation factor Rd. Additional simulations were prepared to address the first question. During the course of this work, an error was found in the original work such that the dispersivities for the results presented were actually a_L = 20.0 ft and a_T = 6.87 ft or a factor of three less than reported. Results for a_L = 60.0 ft and a_T = 20.0 ft have been obtained and are presented in Figs. 32 and 33 and replace Figs. 29 and 30 in the original report. All other conditions in the simulation are exactly as presented in the original report. An additional run was made with a_L =200.0 ft and a_T = 20.0 ft to determine the

sensitivity of the results to the assumed value of the longitudinal dispersivity. These results are provided for ease in comparison in Figs. 34 and 35. One of the original questions which resulted in these simulations is in part no longer valid because the longitudinal extent of the plume increases with the correct dispersivities and 1978-1979 observations are more in line with the predicted plume location. Inspection of Figs. 32 - 35 leave some room for interpretation. Apparently the plume location is a little too far to the south relative to the field measurements, a conclusion that may also be obtained from the previous results. Fig. 33 implies an estimated 10 mg/l contour that has moved downgradient further than implied by the data. On the other hand, the 0.25 mg/l contour location is not unreasonable. This more than likely implies that the source strength was not constant, but in fact was increasing with time. It is possible to conclude that Fig. 35 fits the observed data better than Fig. 33; it really depends upon the interpretation of the available data. Presumably the 1978-79 data are better than the 1975 data and should be used for comparison if for no other reason than the fact that more data is available.

An effort was made to determine reasonable values for the values of retardation factors for phenolics in sandy aquifers. Since this consideration is outside of the author's area of expertise, Dr. Walter Weber of the University of Michigan Water Resources Engineering program was contacted. The result of a personal communication gave an estimate for a distribution

coefficient Kd of approximately 0.91 cm /gm. Since the porosity of the aquifer is necessary to compute the reardation factor through the relation

$$R_d = (1-n)/n \cdot \rho_s \cdot K_d$$

it is only possible to make an estimate of a value for Rd. Table 2 summarizes the computations for a range of realistic values for the porosity. Assuming the distribution coefficient to be approximately correct, these values of Rd are only slightly larger than that estimated from the data in the present study and well within the uncertainty of the estimate. To provide a basis for the interpretation of results, Henry and Force (Dispersion Modeling in Time and Two Dimensions, J. of the Environmental Engineering Division ASCE, Dec. 1979, pp. 1131-1147) states that values of the retardation factor of 27.8 are typical for aquifers. This number is not qualified by aquifer media type and little basis is available for interpretation. Clay media will exhibit stronger adsorption affinity for most organics and it is possible to expect retardation factors to vary considerably for different media types. In view of this discussion, it is still felt that the retardation factor of three is a realistic estimate to within the uncertainties of the other parameters (hydraulic conductivity and the effective porosity) of the Ott-Story aquifer system.

Table 2. Estimated Range of Retardation Factors for Phenols ($K_d = 9.1 \times 10^{-7}$ m^3/gm)

Porosity	Bulk Density (gm/cm^3)	Retardation Factor
0.2	2.1	10.6
0.3	1.86	5.7
0.4	1.59	4.6
0.5	1.33	3.4
NOTE: This assumes specific gravity of 2.65 for media		

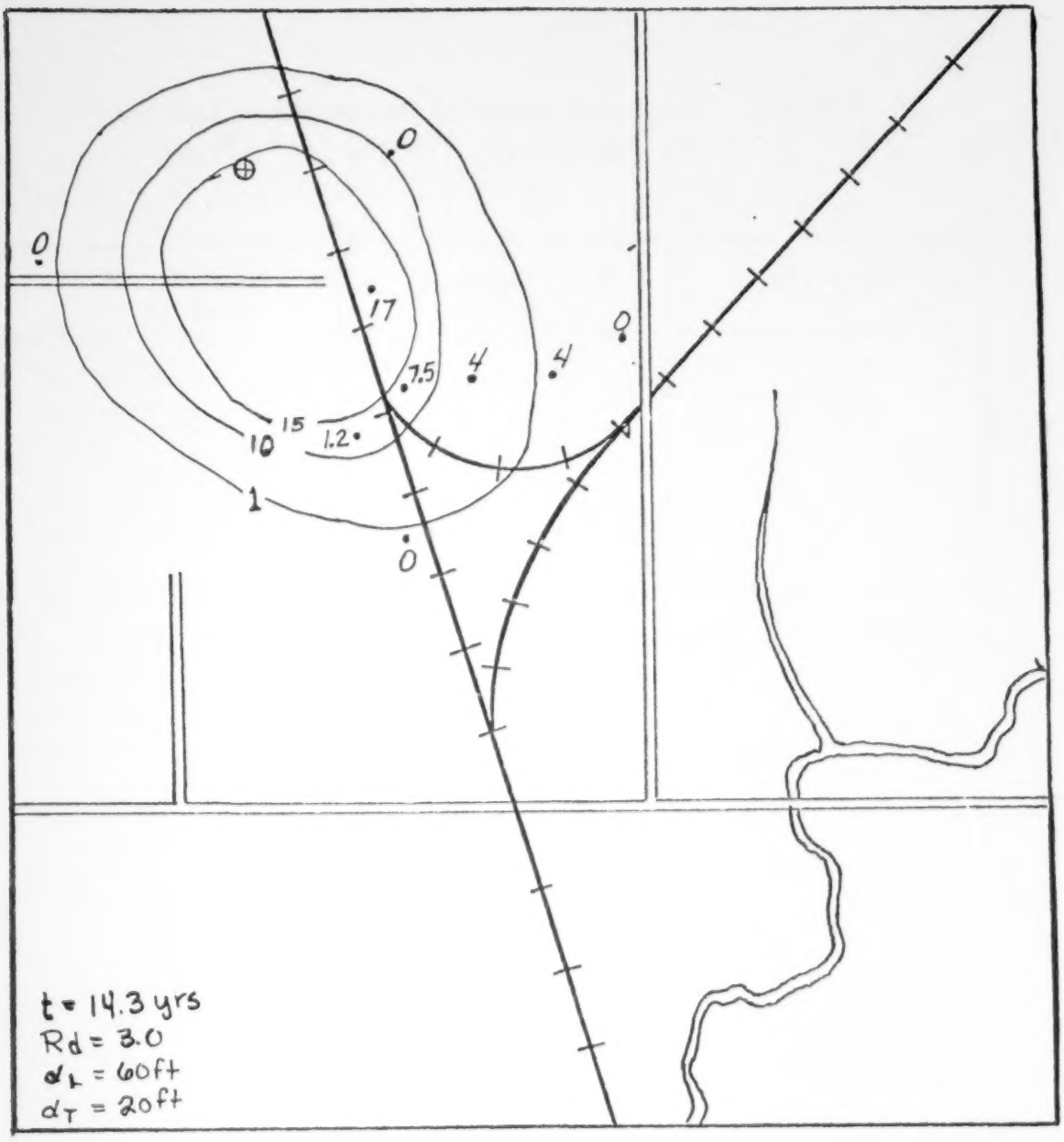


Fig. 32 Comparison of 14.3 year numerical simulation with 1975 Phenol Concentrations (mg/l) (a_L=60 ft)

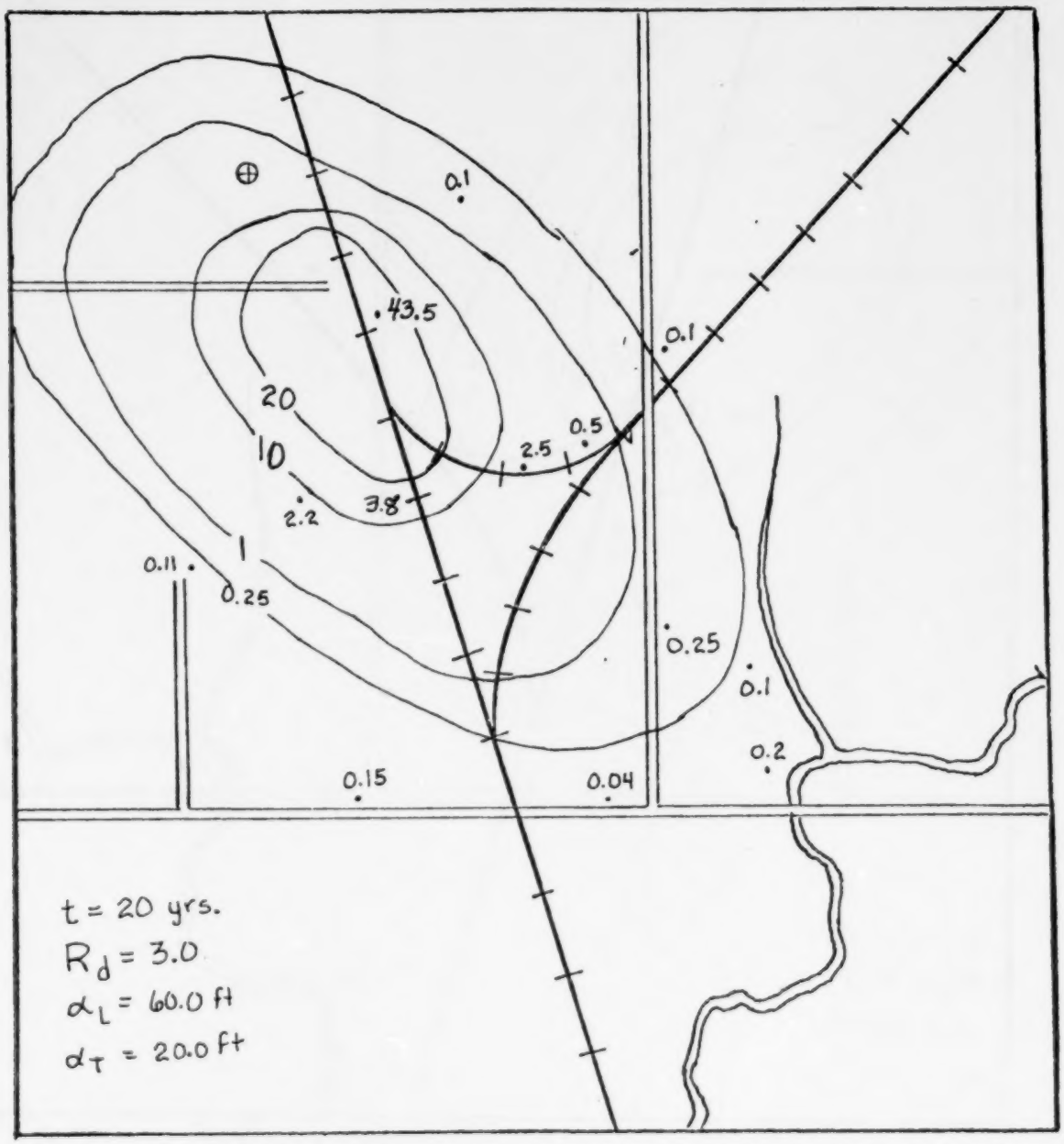


Fig. 33 Comparison of 20 year numerical simulation with 1978-79 Phenol Concentrations (mg/l) (a_L= 60 ft)

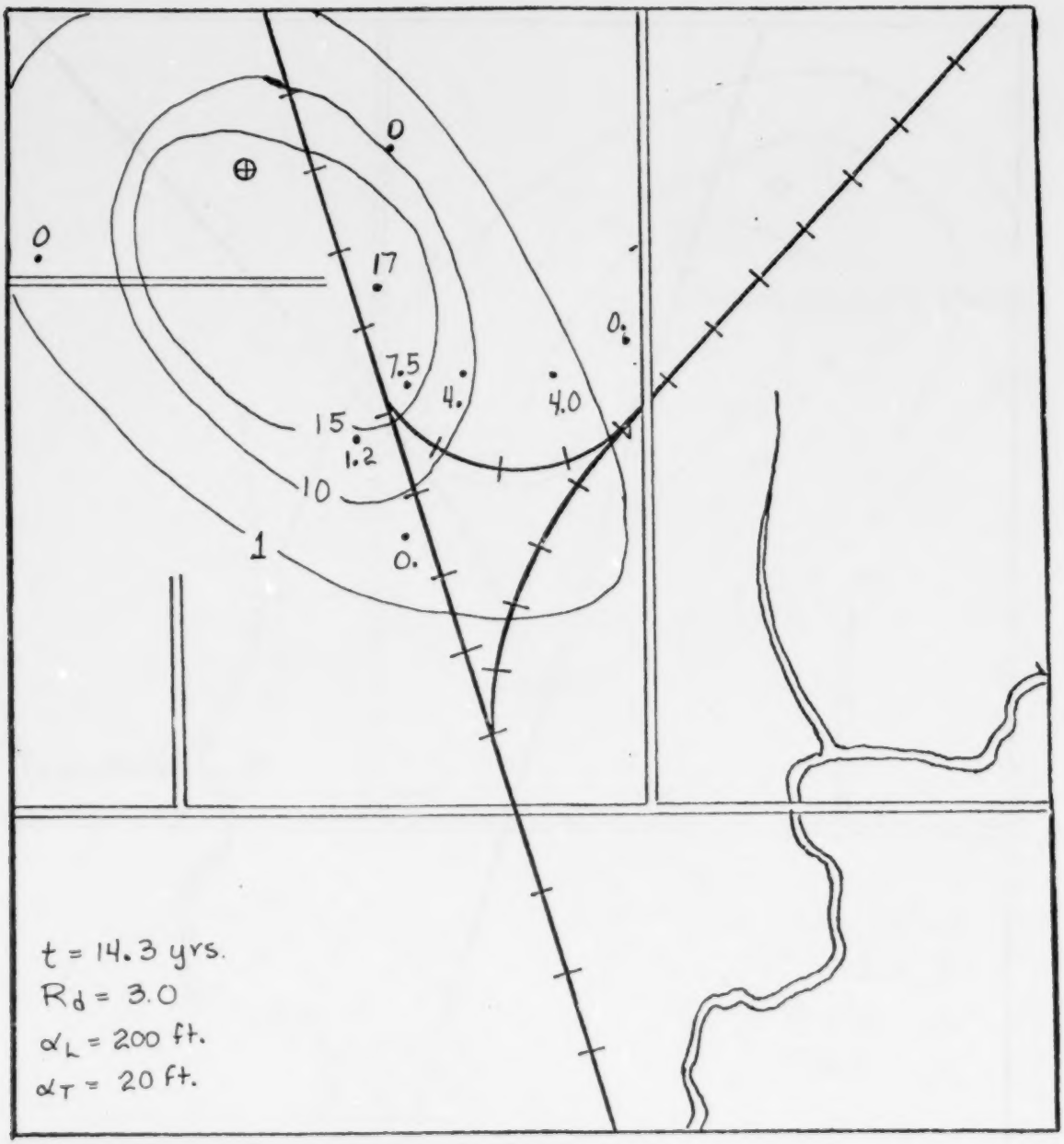


Fig. 34 Comparison of 14.3 year numerical simulation with 1975 Phenol Concentrations (mg/l) (a_L=200 ft)

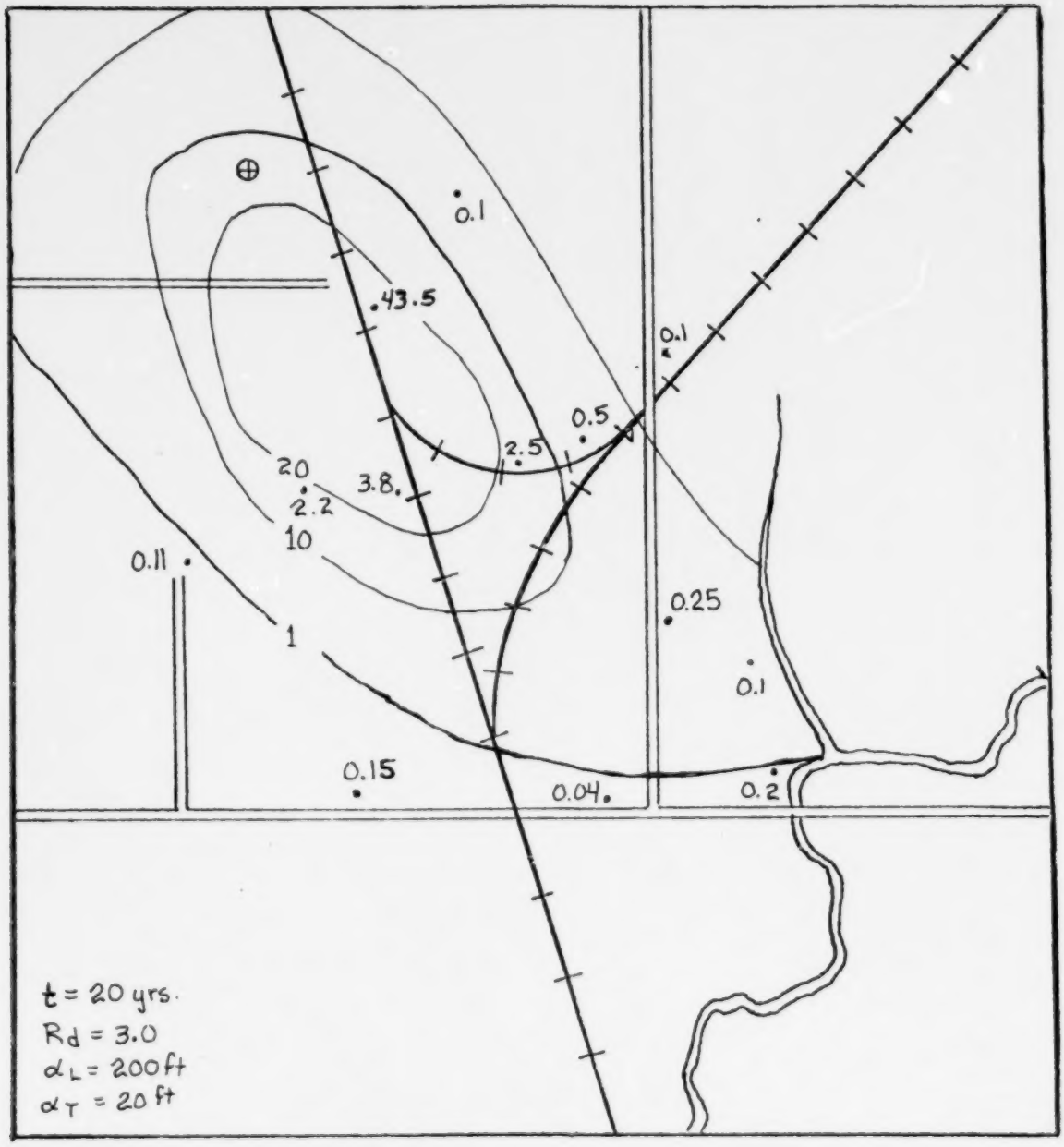


Fig. 35 Comparison of 20 year numerical simulation with 1978-79 Phenol Concentrations (mg/l) (a_L = 200 ft)

APPENDIX C

Aquifer Dispersivities from Field Data - Contaminant Transport in Michigan Aquifers

by

S. J. Wright

AQUIFER DISPERSIVITIES FROM FIELD DATA:
CONTAMINANT TRANSPORT IN MICHIGAN AQUIFERS

BY STEVEN J. WRIGHT

FINAL PROJECT REPORT

TO

MICHIGAN DEPARTMENT OF NATURAL RESOURCES

MARCH 20, 1982

Aquifer Dispersivities from Field Data: Contaminant Transport in Michigan Aquifers

INTRODUCTION

This report is in addition to an interim project report dated July 1, 1981 (Investigation of Contaminant Transport Parameters in Michigan Aquifers) and an addendum to it dated March 20, 1982. The information discussed in the earlier report is not included as part of this report, and only activities considered since that time are described herein. The original contract under which this work was done outlined several possible field sites to be investigated for the purpose of estimating contaminant transport parameters. Included in those was the Ott-Story Chemical site and Wurtsmith Air Force Base. As the study developed, several sites were considered including a styrene spill resulting from a train derailment near Pearl, Michigan. As the investigation developed, this site was eliminated from further consideration due to the local nature of the problem and the difficulties associated an inadequate description of the spill geometry. Three additional sites were ultimately analyzed and are reported herein. These are:

1) A chloride contamination plume resulting from a road

salt stockpile near Indian River.

2) A similar problem at Leverins.

3) A contamination slug apparently due to an accidental spill of chromium at a platins factory at Richland.

The available data was investigated to determine its suitability for the determination of longitudinal or lateral dispersivities from concentration records in observation wells. Since the nature and quality of the data varies from site to site, different approaches to the analysis were attempted in each case. The methods of analysis and results are described herein. Although the results can be obtained through a more rigorous mathematical formulation, the uncertainties associated with the data probably justify the level of approximations employed. It is presently contemplated to perform additional manipulations of the data in a more sophisticated analysis, but little differences in the final results are expected.

Additional objectives of the overall DNR study are addressed in the conclusion of this report. Included are some simulations of contaminant transport at the Richland site. The objectives of these simulations have been developed during continuing discussions with DNR personnel and are described in more detail later. These simulations were performed with the U.S.G.S Method of Characteristics program; an assessment of the capabilites and difficulties associated with the use of the

particular model are discussed. Finally, a summary of the important experiences and conclusions derived from the total investigation are presented to provide the author's perspectives on numerical simulations of contaminant transport.

FIELD DISPERSIVITY INVESTIGATIONS

As in the original report, the author notes the general lack of information regarding the flow characteristics of the various aquifers and the inconsistencies that often exist between the data that is available. Consistent with this observation, it is not good practice under these sorts of circumstances to attempt to obtain contaminant transport parameters by obtaining a "best fit" of a numerical solution to the observed results. Instead, it is felt to be more reasonable to use analytical solutions to simplified longitudinal and lateral diffusion problems which rely upon fewer assumptions regarding aquifer transmissivities, storativities, etc. Although there are errors introduced into the analysis due to the lack of validity of various assumptions, these are felt to be significantly smaller than errors that may be introduced due to improper characterization of the aquifer flow system. A particular approach to the analyses presented herein was dictated by the type and quality of available data. The interpretation of apparent inconsistencies in the data is important is some cases and is justified in the problem descriptions. Each site has been analyzed by a related

approach, although different techniques have been used in each case.

ROAD SALT STOCKPILE CONTAMINATION NEAR INDIAN RIVER

This site is characterized by contamination from an uncovered road salt stockpile that has been exposed to precipitation and subsequent leaching over the years. The contamination plume extended approximately 3600 ft in the longitudinal direction in 1972 and approximately 500 ft in the lateral direction at its maximum width. Water quality measurements, primarily samples from domestic wells, were used to quantify the extent of the plume in the early 1970's and up through the present. remedial action has been taken to control the contamination problem and water quality at the site has begun to improve. Unfortunately, the domestic wells that registered the highest contaminant concentrations, and were abandoned as water supply sources, have not continued to be sampled after they have been abandoned. Therefore, it is difficult to observe the aquifer response over time due to the lack of plume definition. The only adequate data for the purposes of dispersivity determinations is the sampling done in May, 1972. This data has been presented in the form of contour plots for chlorides, calcium, and sodium. All of these show approximately the same plume extent and would all yield approximately the same results as far as plume spreading goes.

The chloride concentrations are generally slightly lower than at the Ott-Story site previously investigated, and while some density effects are probably present, these do not appear to be significant. There are some vertical contaminatnt profiles presented, but these do not provide enough detail to consider vertical effects. The saturated thickness of the aquifer is approximately 100 ft and a two- dimensional horizontal flow assumption is valid except perhaps close to the site. A plot of the chloride profile as estimated in 1972 in a report to the State Highway Comission (Michigan Department of State Highways and Transportation, Interim report of Water Well Contamination Study, Cheboygan County Road Commission, Garage and Environs, Indian River Area, June 15, 1973 and similar report dated January 12, 1972) is presented in Figure 1. The obvious conclusion from an inspection of the profiles is that the source condition probably cannot be approximated as an instantaneous source with constant concentration. This statement is made due to the observation that the "front" of the plume is more than an order of magnitude longer than the width of the plume. If the source could be characterized by a constant strength maintained source, an analytical expression

$$C = \frac{C_o}{2} \operatorname{erfc}\left[\frac{x - vt}{\sqrt{4 a_L x}}\right] \cdot e^{-y^2/4 a_T x}$$

can be applied for a uniform groundwater flow. The water table contours given in the previously mentioned reports are not sufficient to draw any conclusions with respect to the plume

movement; they only imply groundwater movement in the same general direction as the actual plume and a plume location from the extrapolated ground water table would not coincide with the observed plume. If the above solution for a maintained source is assumed to be valid, a plot of the centerline plume concentrations on normal probability paper such as is done in Fig. 2 can be used to easily estimate the longitudinal dispersivity a_L. This approach yields a value of at least 600 ft, depending upon exactly how the data is fit, but the shape of the concentration profile clearly does not support the original hypothesis but instead implies a buildup in the source concentration with time. Therefore, without any information regarding the nature of this buildup, the longitudinal dispersivity may not be estimated from the available data.

There is also considerable difficulty in estimating a lateral dispersivity a_T. Since the plume is not continuous in strength with time, the plume width at a downstream location will be smaller than estimated by a continuous strength at the source. A lateral diffusion solution, such as described previously for the Ott-Story site application is given by

$$C = C_{max} e^{-y^2/4a_T x}$$

Superimposed on Figure 3 is the location of the 100 mg/l choride concentration profile predicted by the above solution and various values of lateral dispersivity. The value of Cmax used is that estimated from the chloride contours. In spite of the limitations in the application, it is clear that a realistic

estimate for a_T lies somewhere in the range of 5-20 ft, with the smaller value a better estimate. An improvement on this attempt can be obtained by solving a convolution integral in time to consider the variable source strength. If it is assumed that longitudional dispersion can be ignored compared to variations in the source strength, a trial and error solution for the source loading can be fit to the observed profile to ultimately estimate the lateral dispersivity. This approach has not been attempted at present because there is not enough independent data to accomplish this; i.e. the source loading determined will not be independent of a_T and vice versa. However, it is possible that only certain ranges of lateral dispersivity will give realistic results. This problem will be considered further in the next few months and an addendum to this report will be filed if anything useful is developed.

Road Salt Stockpile at Leverings

There is very little information available at this site. Basically, the only useful information is the results of a series of tests of domestic wells in 1977 as given in the report of 1978 by Robert Curry to the Michigan Department of State Highways and Transportation (Chloride Contamination of Groundwater, Leverings Area, Emmet County, Sept , 1978). An examination of the report indicates that the local wells either tap the contaminated water table aquifer or a confined aquifer

at greater depth, but no specific information is given on individual wells. Therefore, it is assumed that wells within the plume area that are essentially free of chlorides are in the uncontaminated aquifer. The chloride plume is estimated in the above report by the plot in Fig. 4. It appears from this plot that local effects due to highway de-icing may cause some wells to indicate chloride levels of on the order of up to 50 mg/l. The higher concentrations down-gradient must be attributable to the stockpile. There is clearly a region near the center of the plume where concentrations appear to drop; this is apparently due to a time variation of source input. More than likely, this may be attributable to variations in surface infiltration due to precipitation that varies from year to year. In spite of this, the plume definition is adequate to estimate the lateral dispersivity. Using the same procedure as applied at the Ott-Story site and described in detail in the July 1, 1981 report to the DNR, realistic estimates for at were determined. Cross-sections at the locations indicated in Figure 4 were used to obtain the maximum variations in the estimate of the transverse dispersivity. The plume definition as given in the State Highway department report was used for this purpose. The results of this exercise are given graphically in Fig. 5 and in Table 1. The range in values of lateral dispersivity are from 4.0 to 42 ft. These extreme values are obtained from the data at section 4 as one of the points and therefore should be absolute upper and lower bounds on the estimate by this

procedure. An average value of approximately 20 ft is estimated by this procedure. It is not possible to determine the longitudinal dispersivity from the data available.

It is interesting to note that the three sites studied all yielded approximately the same value for the lateral dispersivity, at least to within a factor of four. It also is of interest to note that they were for fairly similar problems; they were all for aquifers 50-100 ft thick, classified as sandy aquifers, and the contamination problems had roughly the same magnitude of chlorides. This more or less supports the concept of being able to apply results from one aquifer to another one that is similar, at least when the problem is on a regional scale. It is possible in all of the situations analyzed that the dispersivity is somewhat overestimated. Reasons for a systematic overestimate may be:

1) Although density effects may be small, they may cause additional spreading in the lateral direction

2) The plume contours provided probably overestimate the plume extent. In all cases, the contours that are used to depict the plume extent are systematic in that, for example, the person drawing in a contour (e.g. the 250 mg/l contour) will nearly always encompass all wells which indicate all samples which have a higher concentration than the contour level. This often results in many readings less than the contour level also falling within the contour extent and does not reflect a true

average contour location.

3) Related to this consdideration is the fact that no data giving a lateral profile at a particular location is available. It is reasonable to expect that if this detail were available, the plume boundary would be found to shift around more in the lateral direction with a narrower actual width.

In spite of these considerations, it is logical to use the estimated values of tranverse dispersivity, rather than the true ones, in any numerical simulation of a regional aquifer problem. This is precisely because density effects are generally ignored in two dimensional simulations and it is also generally desirable to know the probable maximum lateral extent of the contaminant plume which does involve all of the unknown flow path variations that have not been considered in the above analyses.

Chromium Contamination at Richland

The discussions immediately above is partially intended as a preface to the presentation of these results since the data for this site are significantly different than for the three previous sites. The fact that individual observation well data (point data) is analyzed here more than likely results in lower estimates of dispersivity due to the reasonins presented in explanations 2 and 3 above. The implication may well be that

the regional problem should be analyzed with a somewhat larger dispersivity than extracted from the data, but the slug nature of the contamination problem in this particular instance has its own implications.

The source of the contamination at this site is assumed to be from a chromium spill at the Production Plated Plastics plant site which is upgradient from the observed contamination. The specific data available is a series of Public Health Department analyses of domestic wells for chromium, partial results of a hydrogeological study by Keck Consulting Services of Williamston, Michigan, and several DNR memos regarding the problem. Several of these wells show high chromium concentrations, especially those wells labeled V-1, WM-1 and WG-1 as indicated by locations in Fig. 6. Also indicated is the plant site and the location of a known spill observed during a DNR inspection of the plant site. Keck Consulting Services' hydrogeological investigation of the site, including soil sampling, installation of some monitoring wells and determination of the local groundwater table. Their investigation shows the plating plant to be directly upgradient from most of the sites with high chromium concentrations including well G-1 which is some distance away from the other wells. However, the source for well G-1 would have to be at a different location than for the others. Apparently, the problems in well G-1 are related to some other incident and not related to the conditions in the other wells. From the time

records of the chromium concentrations in these various wells, reasonable estimates of the longitudinal dispersivity may be obtained. On the other hand, there is insufficient information to estimate the lateral dispersivity although a range of values can be bracketed. For this particular problem a point source solution for a uniform groundwater flow is assumed to be valid

$$C = \frac{M}{B} e^{-\frac{(x-vt)^2}{4a_L x}} \cdot e^{-y^2/4a_T x} \cdot \left\{ \frac{1}{4\pi x \sqrt{a_L a_T}} \right\}$$

where M is the source mass and B is an average aquifer thickness The dispersivities may be estimated by fitting normal distributions to the observed concentration profiles and by making various simplifying assumptions regarding the nature of the groundwater flow that can be extracted from the available data. Plots of the time history of chromium concentrations in the four wells G-1, V-1, WM-1, and WG-1 are presented graphically in Figures 7-9. Since the latter two wells appear to be along the prevailing flow path, and the general shapes of the profiles are the same, they are combined in Fig. 9 with a time shift to account for the difference in flow time between the two locations. The point source solution can be used more readily in a regression analysis if it is assumed that no dispersion occurs as the slug moves past a particular site. In this case, the solution is rewritten as

$$C = C_{max} e^{-\frac{(x-vt)^2}{4a_L T}}$$

where T is an average "time of travel" (i.e. the time for the peak to travel to the region of interest). Since there is so

little dispersion in this problem, this is a reasonable approach. Seepage velocities are estimated by the time of travel of the peak concentration between the three wells and the Keck observation well OW-12. The results of these estimates are included in Table 2 and indicate a seepage velocity of approximately 1.25 ft/day. This number is used in all subsequent computations.

The profiles in Figs. 7-9 were fit to a profile of the form

$$C/C_{max} = e^{-bt^2}$$

t is time from the peak concentration

where b is to be determined by some best fit process. A linear regression (between $\ln(C/C_{max})$ and t^2) to compute values of b resulted in the tails of the distribution being weighted a little more heavily than visual attempts to best fit the distribution. The linear regression results are summarized in Table 3 along with the computed value of the dispersivity with the other parameters as estimated. Note that a visual best fit process would eliminate the small "bump" on the leading edge of the distribution (data from wells WM-1 and WG-1) and would give values for longitudinal dispersivity more in line with the other results. It appears likely that the actual spill conditions may result in this deviation from a normal distribution and any deviation from a true point source will result in larger estimated values of a_L. Therefore, it is to be expected that the values given are likely to be upper bounds on the true value

of the dispersivity.A value for longitudinal dispersivity of 2 ft would be a fairly realistic choice for this particular problem. Although this is considerably smaller than the values estimated previously for lateral dispersivities, part of the reason may be the fact that the estimates in this case are from point measurements and all of the effects of using a number of wells to define a plume are not considered. In general, it should be anticipated that longitudinal dispersivities should be greater than lateral ones in a given aquifer so long as the medium is isotropic. Since the travel distances are not significantly different than the other sites considered and the gross aquifer characteristics are not apparently much different, perhaps it should be concluded that the medium is more homogeneous than in the other cases.

Any estimate of lateral dispersivity is only an order of magnitude estimate based upon an assumed flow field in the vicinity of the contaminant slug. If the water table contours from the Keck hydrogeologic investigation are assumed to be correct, wells V-1, WM-1, and WG-1 are essentially along a streamline with a deviation of only 100 ft or so in a lateral direction. On the other hand, the Keck water quality samples show both OW-12 and OW-13 with significant chromium concentrations. These are separated at least 650 ft in a lateral sense. Deducing a longitudinal conentration profile from the three wells in Figs. 8 and 9 implies that it took approximately 550-600 days for the bulk of the slug to pass a

point only slightly upgradient from OW-12. Multiplying this by the estimated seepage velocity of 1.25 ft/day yields a longitudinal dimension of approximately 700 ft. In this case, the lateral dimension must be at least that much and probably more. Since there is no definition of the source discharge available, it is hard to say how much of the lateral effect to attribute to the source effect and how much to dispersion. Without a extremely unusual circumstance, it seems unlikely that the source would be an order of magnitude wider than it is long. If the lateral dispersivity were, say, 0.2 ft, four standard deviations for 2000 ft of travel would only be 113 ft and all of the lateral effect would be essentially due to source conditions. Therefore on this basis, a tentative conclusion may be that lateral and longitudinal dispersivities are approximately equal for this situation. Although this argument is not based upon much data, it seems to be plausible unless any information to the contrary is developed.

NUMERICAL SIMULATIONS

As part of the overall study objective, numerical simulations were performed for this site. Purposes of this phase of the investigation were to evaluate the capabilities of numerical models in terms of reproducing a known contamination problem. Since considerable effort was expended by others in simulating the flow conditions, very little time in this study

was spent towards that end. Results as obtained in simulations by David Hamilton at the DNR were used to develop the flow models. Runs were made with the U.S.G.S. model for both a small and large grid. The small grid covered essentially only the areas where the chromium data was available and consisted of a 125 ft long by 125 ft wide spacing between nodes over the region depicted in Fig. 10. The larger grid covered most of the known groundwater flow system and consisted of nodes on a 500 ft by 250 ft spacing as in Fig. 11. Elevations of the aquifer bottom were estimated from the DNR simulations and variedsomewhat between the two grids; Fig. 12 shows the elevation contours for the large grid. Water table elevations from the previous simulations are used as boundary conditions for these simulations; output from the simulations are included as part of this final report and the exact conditions may be obtained from those. Water table contours computed for the small grid are given in Fig. 13 and similar results for the large grid are presented in Fig. 14. A variety of related runs were made and are summarized in Table 4. Results for the larger grid are not sufficient in resolution to compare field observations against, particularly at the smallest dispersivities. On the other hand, the small grid did not extend far enough to predict future plume movement. The results of some of the simulations are presented in Figs. 15-19. Figure 15 contains the predictions of the plume migration predicted with the small grid. Included is the trajectory extrapolated from the computed results and peak

values at selected times. Also included is a concentration profile at a particular time when the slug is in the vicinity of the observation wells. concentrations are relative to an arbitrary source value of 1000 and do not represent an absolute measure of concentration. Since the peak plume trajectory is away from the observation wells, it is impossible to make a reasonable estimate of the actual peak concentration. There are so many uncertainties is the simulation including the assumed source location that it is not logical to attempt to do so. Note the the USGS model does not necessarily predict continuously decreasing peak concentrations with time. This is due to the fact that the concentration peak can lie in between nodes and be averaged out over several, whereas at a later point in time, it can be more or less aligned with a single node. Fig 16 is a simlar plot with the large grid siulation results. Fig. 17 was an attempt to compare the results of D. Hamilton's analytical solutions for the site. The comparisons are not good for two major reasons. First of all, the numerical simulations predict velocities less than 1.4 ft/day in the upper portions of the grid and therefore the slug lags behind the analytical solution with a constant velocity of 1.4 ft/day. Also, the USGS model distributes a source over an entire nodal area, 500 ft long by 250 ft wide in this case. The analytical solution only has a 126 ft long (90 day x 1.4 ft/day) source. The question of comparison with analytical solutions is raised again below with a different problem which is a better test case. Fig. 18

compares the results of a slug that lasts 100 days versus the instantaneous source in all other solutions. Since the resolution of the large grid is not very good actual output concentrations at the various nodes are provided rather than trying to plot contours. Fig. 19 is an attempt to predict the present location of the slug. Graphical results are not presented for the two pumping runs. For the two pumping rates of 250 gpm and 1000 gpm, the purge well, as located in Fig. 19 would successfully capture all of the contaminant for the dispersivities used. The lateral dispersivity of 1.5 ft is the most critical issue in this respect. Comparison of the various results discussed above seems to show a smaller width for the slug than might be expected from the OW-12 and OW-13 results discussed earlier. However, the longitudinal dimensions of the slug are better reproduced with the 1 ft dispersivities. The best that can be deduced here is that probably similar values for lateral and longitudinal dispersivities are logical for this problem. Obviously before any attempts are made to install an actual purge well system, further monitoring should be done to resolve some of the questions outlined in the section of dispersivity estimates.

SUMMARY AND CONCLUSIONS

A number of separate issues are addressed below; these are discussed separately.

Estimates of Dispersivities

It is felt that realistic estimate of field dispersivities have been obtained in this study. Consultation of the literature yields a wide range of values depending upon the methodology employed. The paper by Pickens and Grisak (Water Resources Research, August, 1981) gives a good summary of several previous studies. Generally, dispersivities estimated by fitting data by numerical solutions are larger than those obtained in the present study. This is to be expected, since the numerical solutions effectively require the dispersivity to make up all of the ignorance in actual source conditions; this is especially so with longitudinal dispersivities. On the other end, pumping tests often result in lower disperstivities than computed herein. This can be expected for two reasons; 1) the relatively smaller scale of the experiments and 2) the fact that these are point measurements. The implications of this second factor was discussed above and the first simply reflects the known condition that disperisiviries exhibit some dependence upon the physical scale of the system (Pickens and Grisak suggest the longitudinal dispersivity to be a linear function of distance at small scales). Thus, the values obtained fall

generally within a range that may have been anticipated at the outset of the investigation, although the results for the Richland site may be somewhat low for what might be expected. When considerations are made of the relative uncertainties of the estimates of these quantities and the implications as compared to the uncertainties, for example, in hydraulic conductivities, it is clear that any dispersivity of the correct order of magnitude should be acceptable in a numerical simulation. Given this consideration, the results of this study should be applicable to other related sites in the state, at least for circumstances where data is not available from which to make an estimate.

Modeling Philosophy

For problems of the type considered in this study (regional aquifer problems), a few conclusions seem justified from the study results. The major point is that estimates of hydraulic conductivity from well tests (as at Ott-Story) or lab tests (as at Richland) are the single largest impediment to numerical modeling of contaminant transport. In each of these two cases, if a modeling objectiive was to predict plume location as a function of time, the results would have been off by approximately a factor of two if the supplied estimates were used. Considered within this framework, the choice of dispersivity is unimportant except, of course to ultimate plume

extent. But in regional aquifer problems with travel distances of 1000 ft or so, the spreading is not that important relative to the need for accurate flow simulation. Therefore, a strong consideration should be made as to whether a contaminant transport model is really required in a specific application. If it is felt to be, the use of approximate analytical solutions are probably reasonable for many circumstances and the effort of a complete transport analysis is not justified except under extreme circumstances where sufficient data is available to make good estimates of all necessary parameters or where geometries are very complicated.

Model Assessment

The U.S.G.S. Method of Characteristics model was felt to be fairly accurate for the problems that were investigated in this study. Very little numerical dispersion was apparent in the computed results; this, of course is the primary selling point of the particular model. It is interesting to compute numerical Peclet Numbers for the typical problems encountered in this study

$$P_e = \frac{V \Delta x}{D_h} = \frac{\Delta x}{a_L}$$

Values for the Peclet number significantly greater than unity imply advection dominated problems; these conditons must always occur for the regional type of aquifer problems with grid sizes

of several thousand feet and dispersivities of at most tens feet. The implication of this consideration again reinforces the conclusion above; the flow field computation is most important. Given these considerations, the U.S.G.S. model should be well suited to problems of the regional aquifer type. A better demonstration of the numerical capabilities of the model is obtained with a comparison of a more well defined problem. A uniform groundwater flow of 2 ftt/day is simulated with a 25 ft wide source at one upstream side of the system. The computed results are compared with an analytical solution to the same problem 100 days after the beginning of the source in Fig. 20. The comparisons are quite good except near the source. This is again due to the fact that the USGS model distributes sources over entire nodes, and also partially due to the fact that concentrations are averaged over nodes. Only is the concentration is linear with distance will the average nodal concentration be equal to the concentration at the node midpoint. The form of the analytical solution would imply the shift of the 0.8 contour in the sense indicated by this latter explanation; the influence can only be minimized by making the grids finer and finer.

The only problems noted in the various solutions were associated with runs where the ratio of longitudinal to lateral dispersivity was 10 or more. Under all of these circumstances, negative concentrations began to appear at the edges of the computed plumes; these are not suppressed in the computations.

The magnitude of the negative values was always much less than the magnitudes of the maximum concentrations, but it is not clear that this problem would not become worse under certain circumstances.

There were many practical problems with the implementation of the numerical code. One problem was with the explicit nature of the code and the fact that the computational time step is set internally within the program. In the vicinity of pumping wells, the flow velocities can be very high and the computational time step correspondingly small, requiring an excessive number of calculations to cover a given simulation period. This situation is problem specific, but should be considered in the problem formulation to avoid excessive costs associated with a particular simulation. Another problem that is not specific to the particular numerical code is the lack of computational resolution for small travel distances. This was especially true for the Richland simulation and necessitated going to the smaller grid. This problem will arise in any numerical code that requires a constant grid size. At least the small size of the slug in a large grid does not create serious computational inaccuracies with the U.S.G.S. model. Finally, problems arose in specific applications with the model. The model is not set up to compute an intial steady state, so any transient calculation first requires a separate simulation to set a reasonable initial condition. The code will allow steady state flow solutions, but simply doesn't allow starting a

transient calculation from a computed steady state. This would represent a significant improvement in the model. Other than that, the code is somewhat limited in the number of options that are available, but does have the capabilities necessary to solve most commonly encountered problems. Some of the procedures to be followed are a little obscure and a certain amount of familiarity with the code helps in the setup of problems. The manual is not very well written, but all of the information is there somewhere.

Table 1. Estimates of Lateral Dispersivities at Levering, MI from Chloride Plume

Section	x ft	σ ft	a_T			
			1-	2-	3-	4-
1	115	91				
2	333	124	16.3			
3	960	213	21.9	23.9		
4	1900	150	4.0	--	--	
5	3000	338	18.4	18.5	16.9	42.0

Table 2. Estimates of Seepage Velocities from Time of Travel of Chromium Slug at Richland, MI

Wells	Distance (ft)	Time(Days)	Seepage Velocity ft/day
V-1: WM-1	344	275	1.25
WG-1: WM-1	100	73	1.35
V-1: OW-12	750	730(est)	1.03

Table 3. Estimates of a_L from time Histories of Chromium in Observation Wells at Richland, MI

Well	Assumed x(ft)	b $days^{-2}$	a_L
V-1	1500	1.4×10^{-4}	1.86
G-1	2600 3250	5×10^{-5}	3.00 2.40
WM-1, WG-1	1875	1.6×10^{-5}	13.0
NOTE: Seepage velocity used in computation was 1.25 ft/day			

Table 4. Summary of Different Computer Rums for Richland Site

Grid	a_L (ft)	a_T (ft)	Time (Years)	
Small	1.0	1.0	6.0	Instantaneous
Small	5.0	5.0	6.0	
Large	1.0	1.0	12.0	
Large	5.0	5.0	12.0	
Large	1.0	1.0	12.0	100 Day Source
Large	5.0	1.5	8.7	
Large	1.0	0.29	8.7	
Large	5.0	1.5	6.0	Purge Well 250 gal/m
Large	5.0	1.5	6.0	Purge Well 1000 gal/min

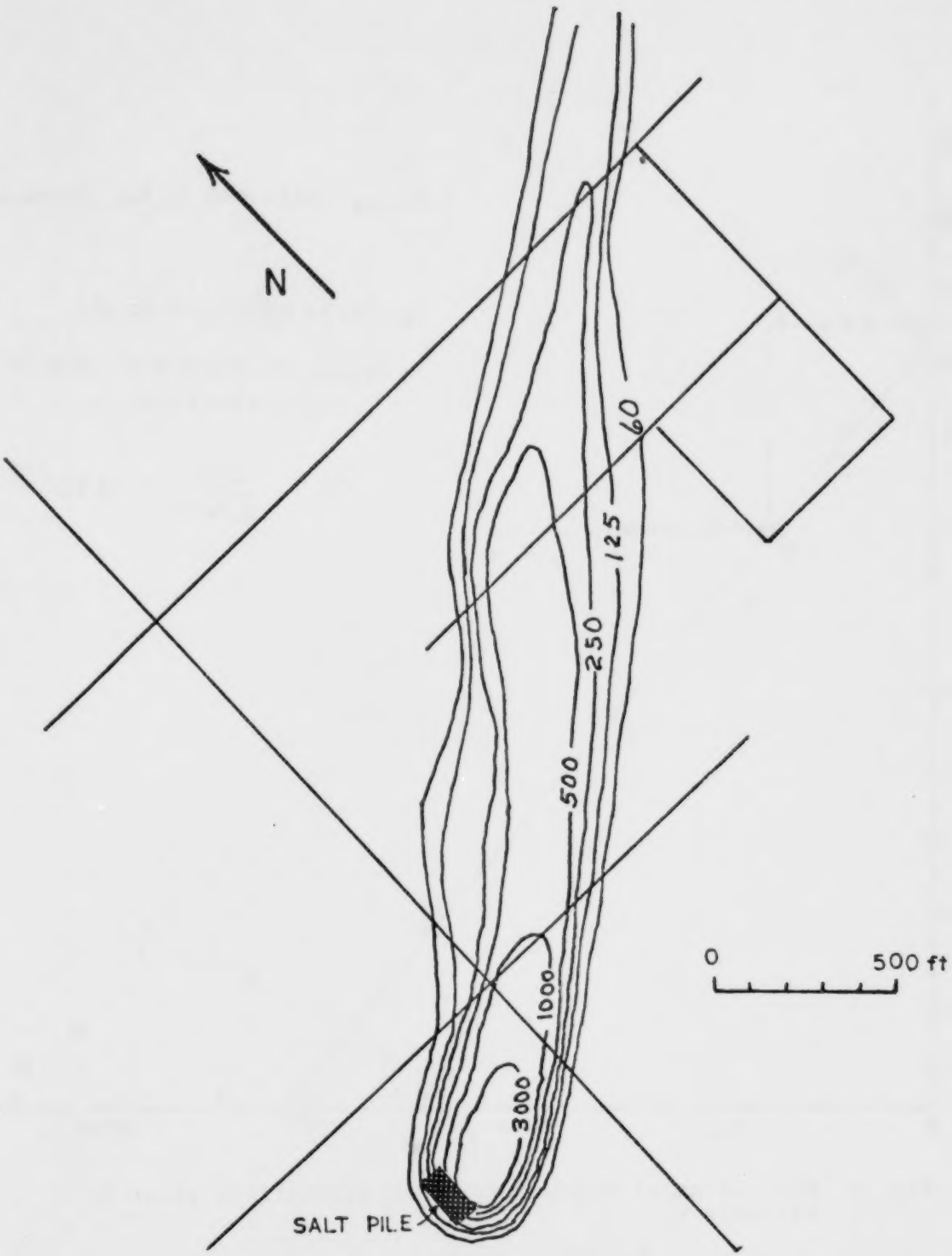


Fig. 1 Estimated May, 1972 Chloride Plume at Indian River

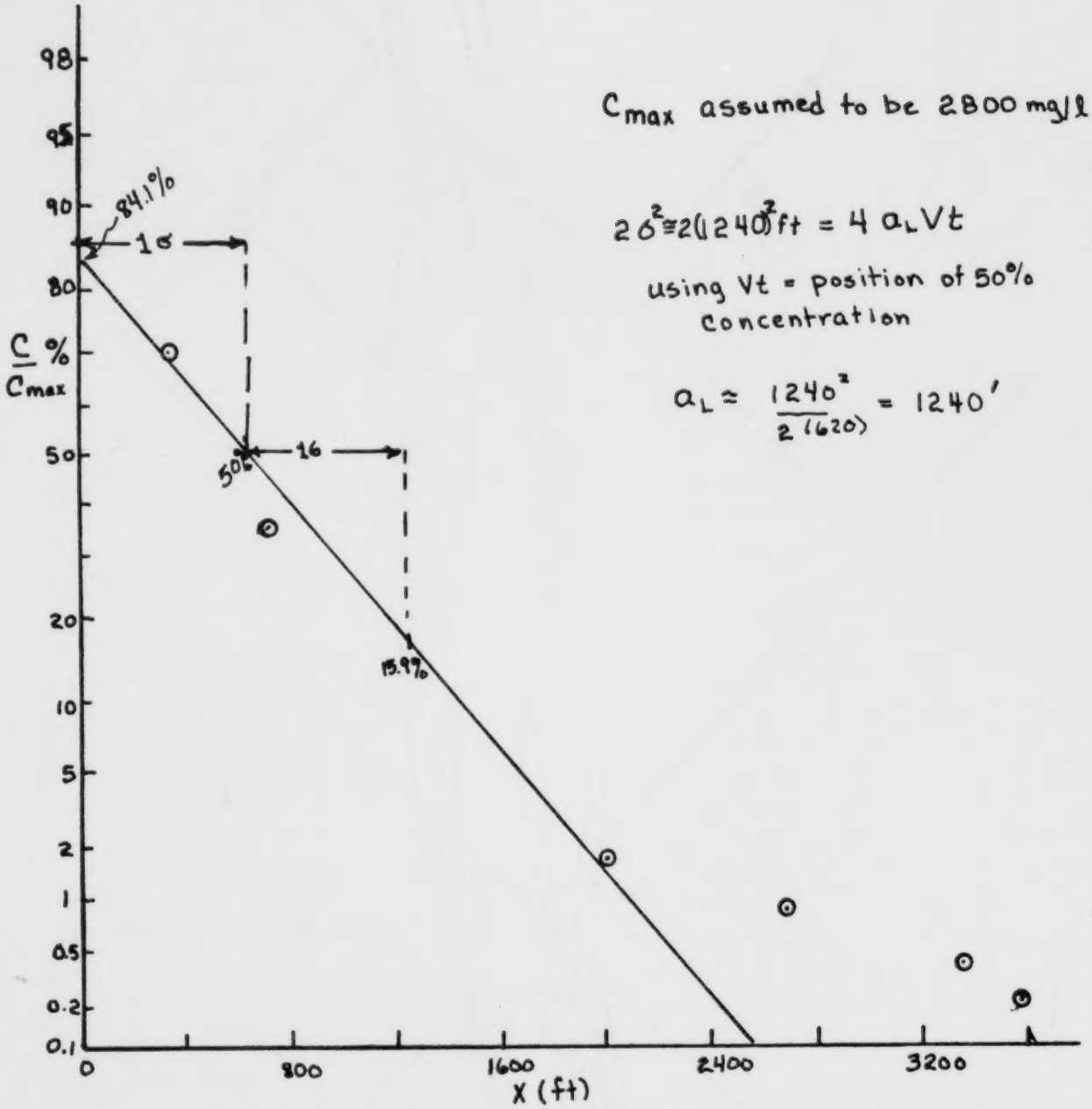


Fig. 2 Plot of axial concentration on probability paper to estimate a_L

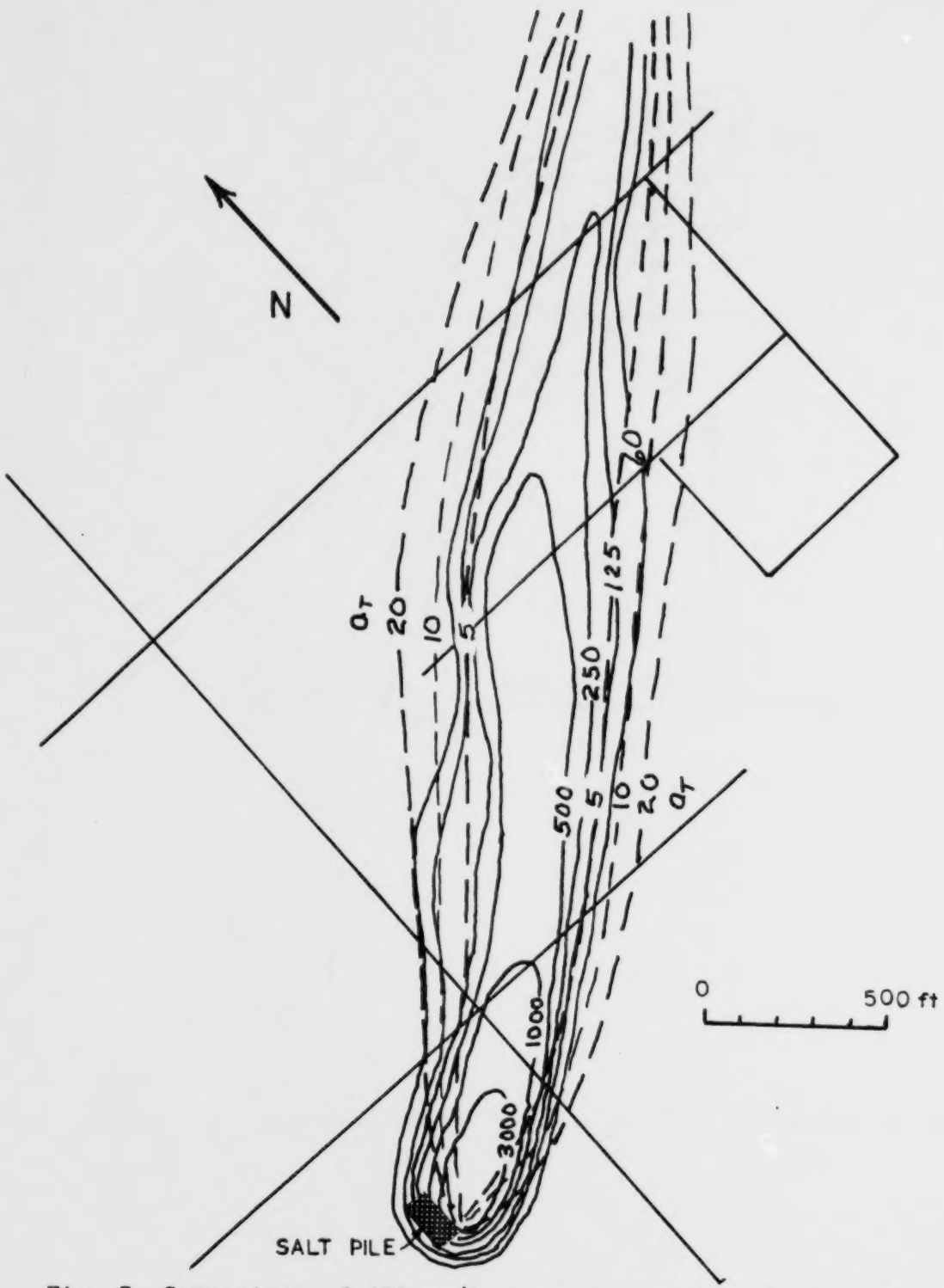


Fig. 3 Comparison of 100 mg/l contour on Indian River Chloride Plume with predictions for several a_T values

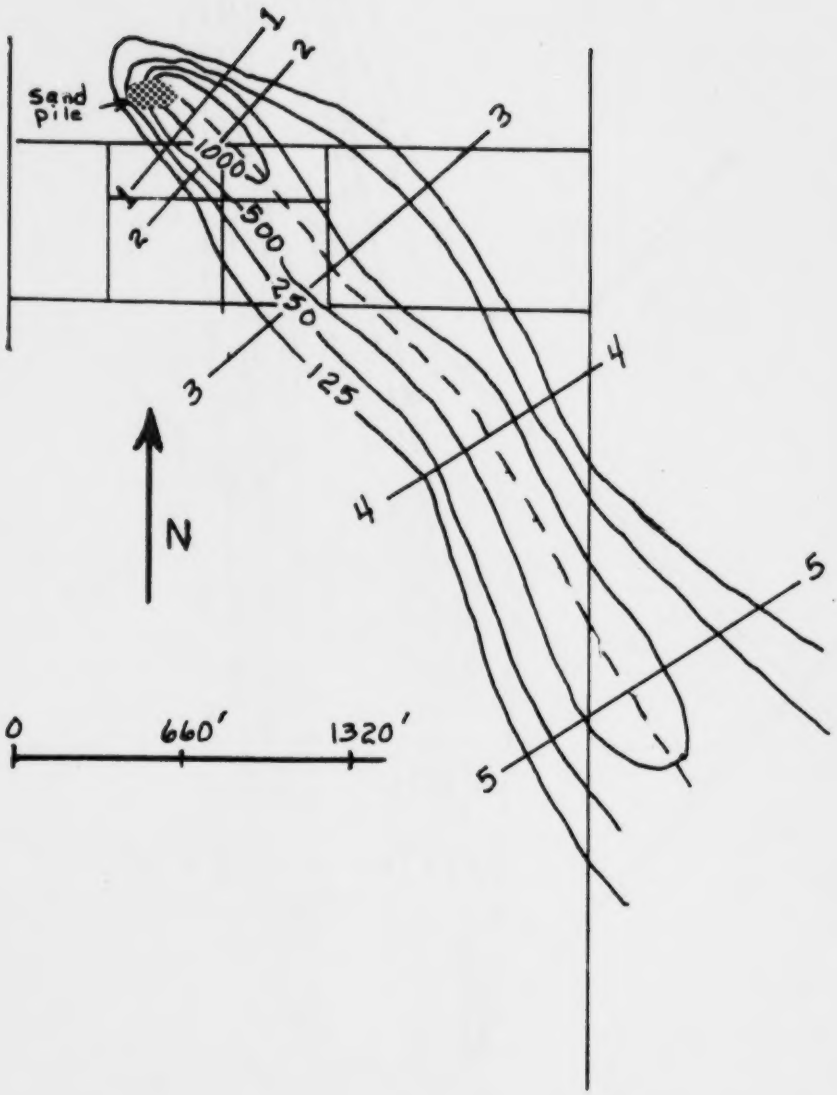


Fig. 4 Estimated 1977 Chloride Plume at Levering

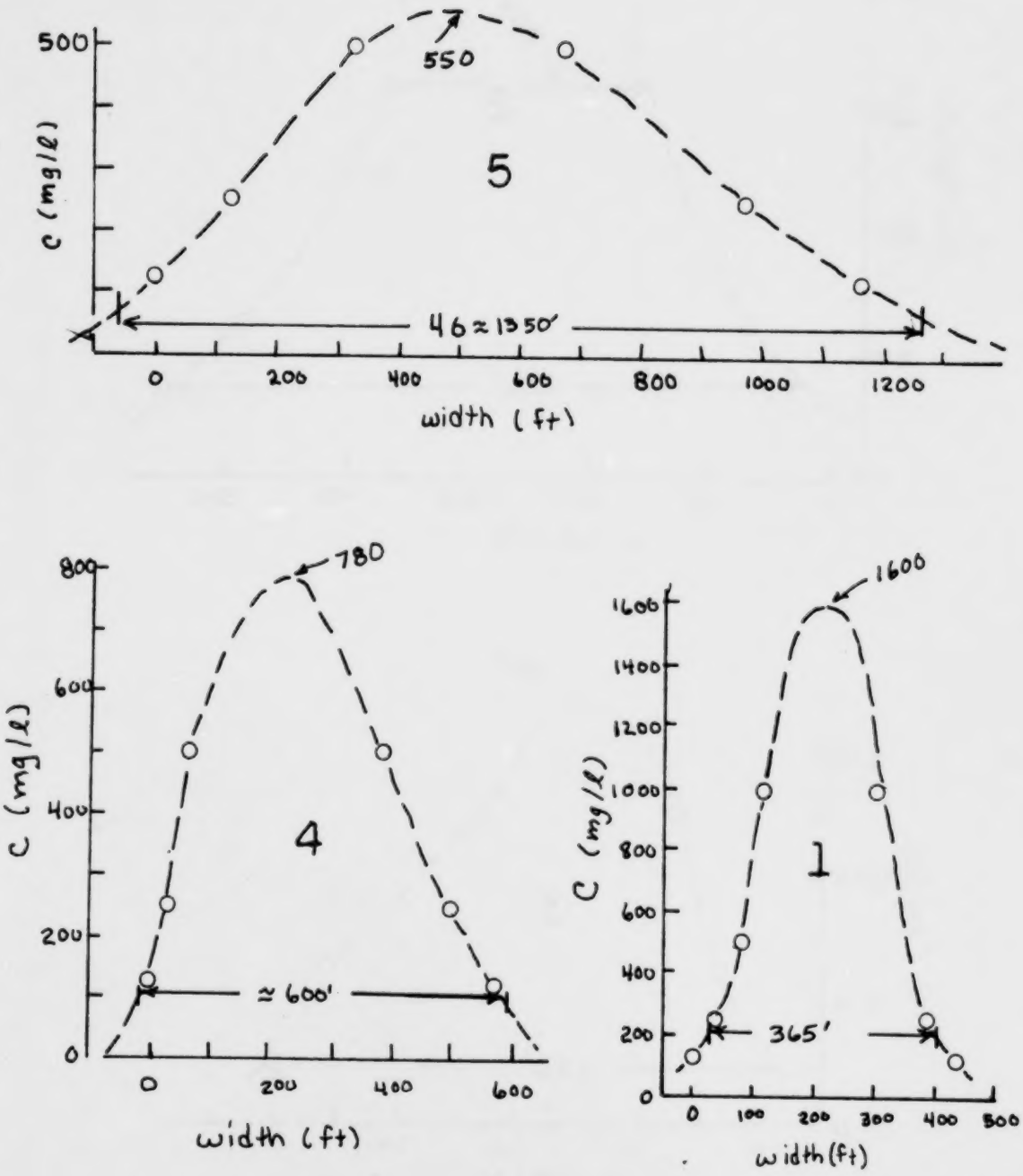
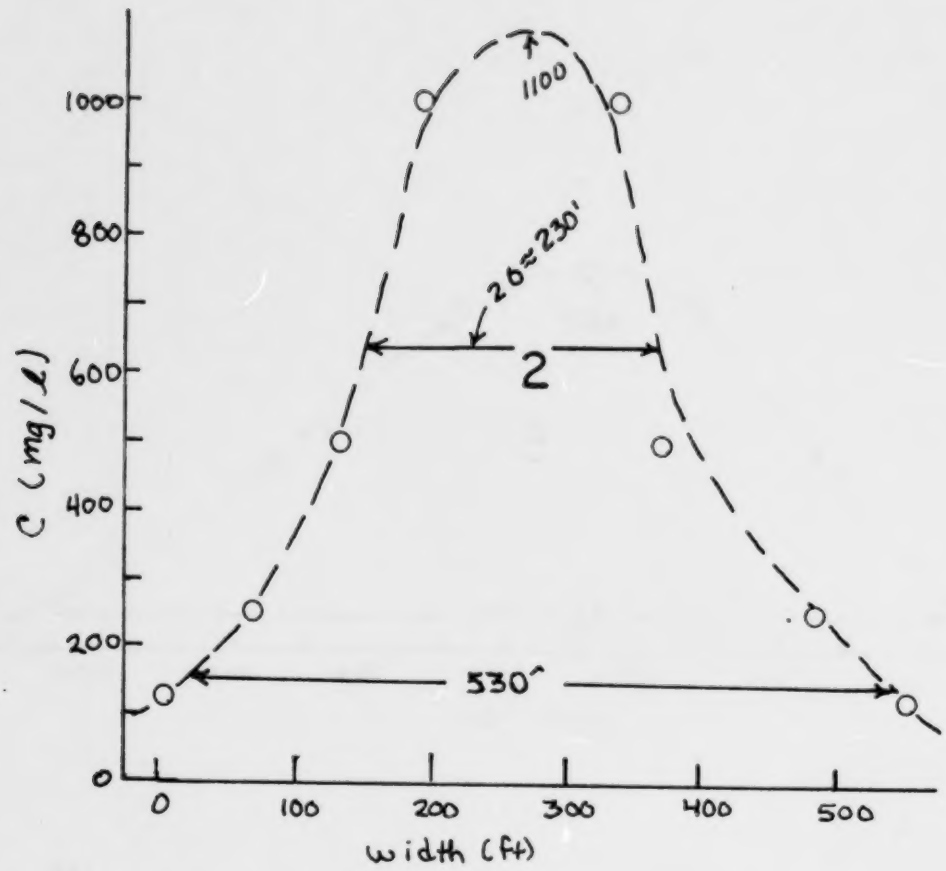


Fig. 5a Lateral Concentration Profiles in Levering Chloride Plume



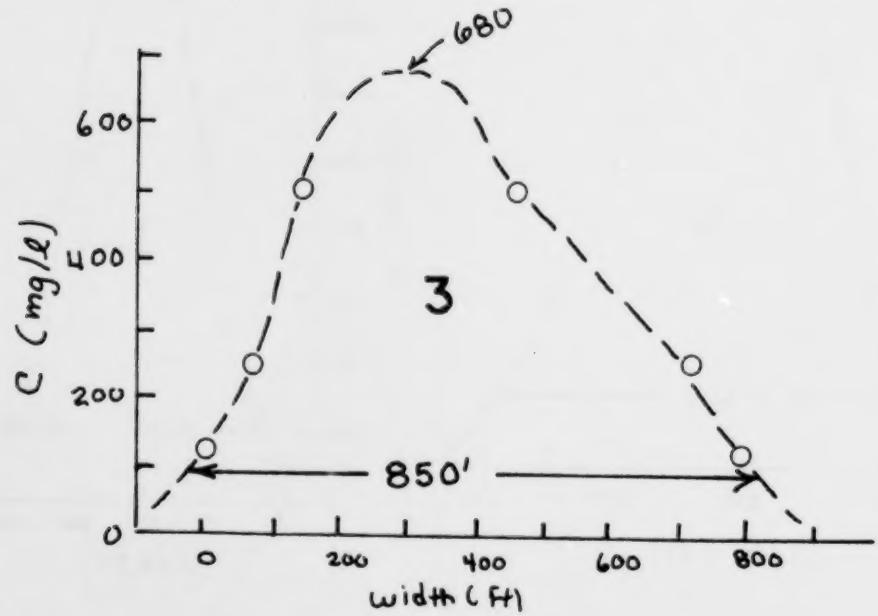


Fig. 5b Lateral Concentration Profiles in Levering Chloride Plume

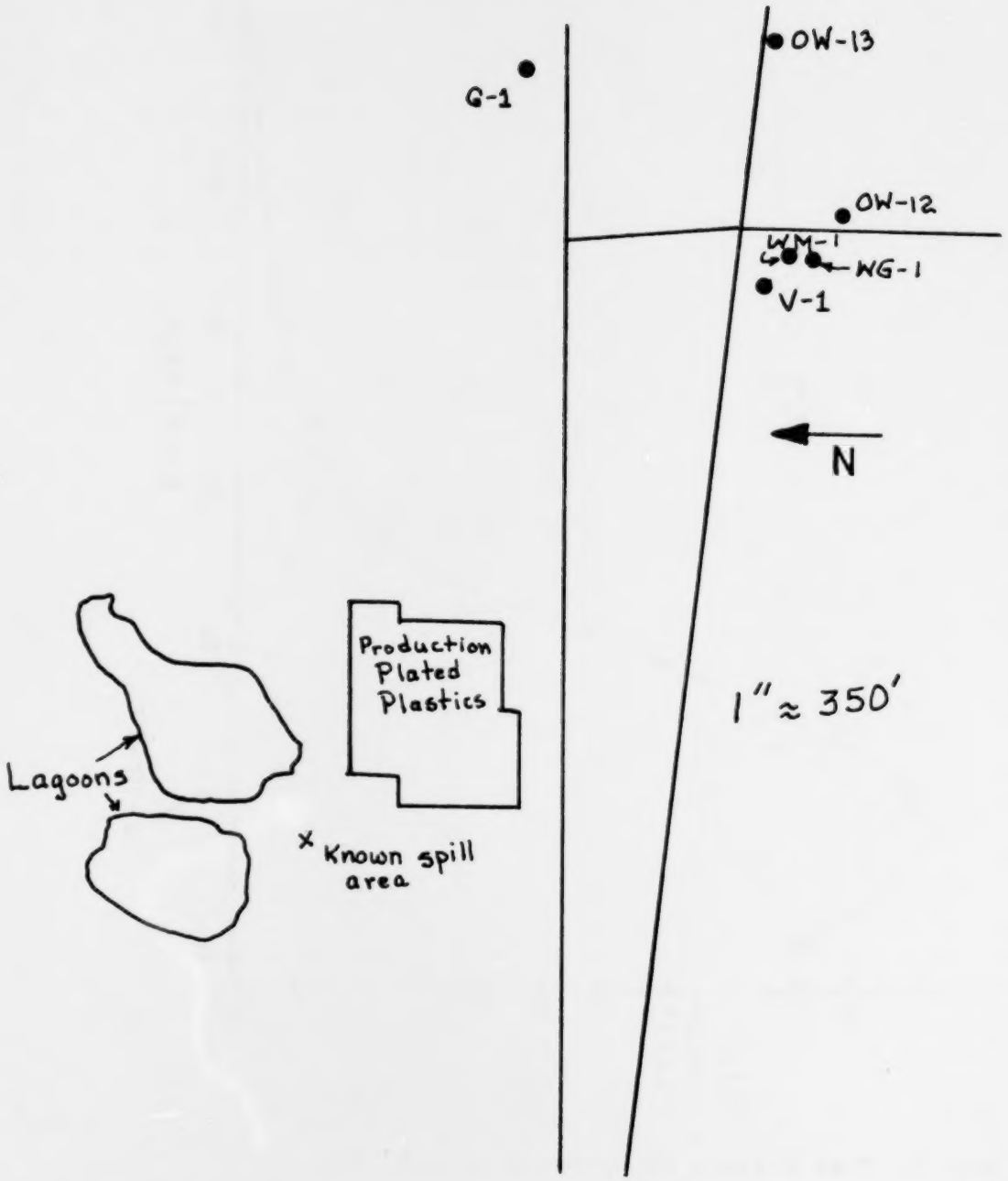


Fig. 6 Site Map at Richland with Observation Well Locations

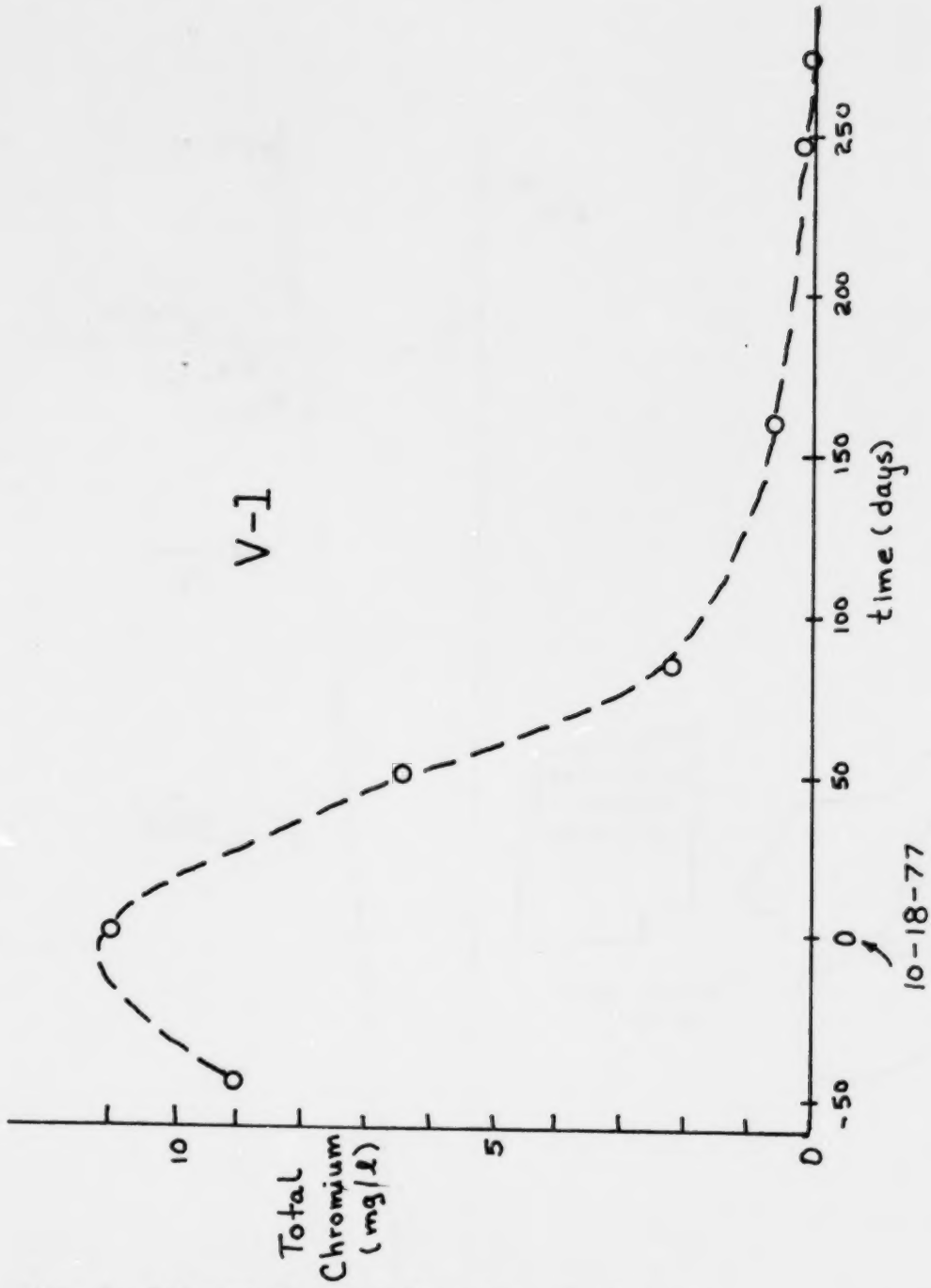


Fig. 7 Time History of Chromium in well V-1

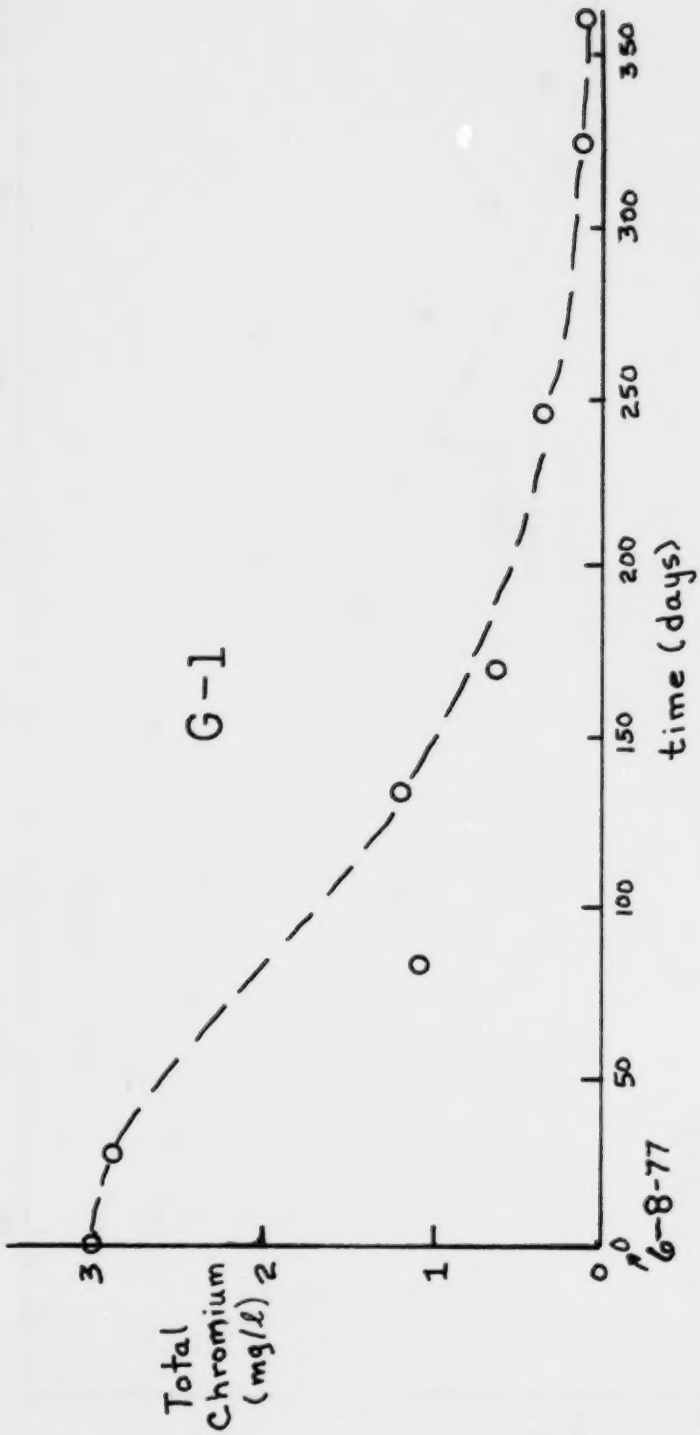


Fig. 8 Time History of Chromium in well G-1

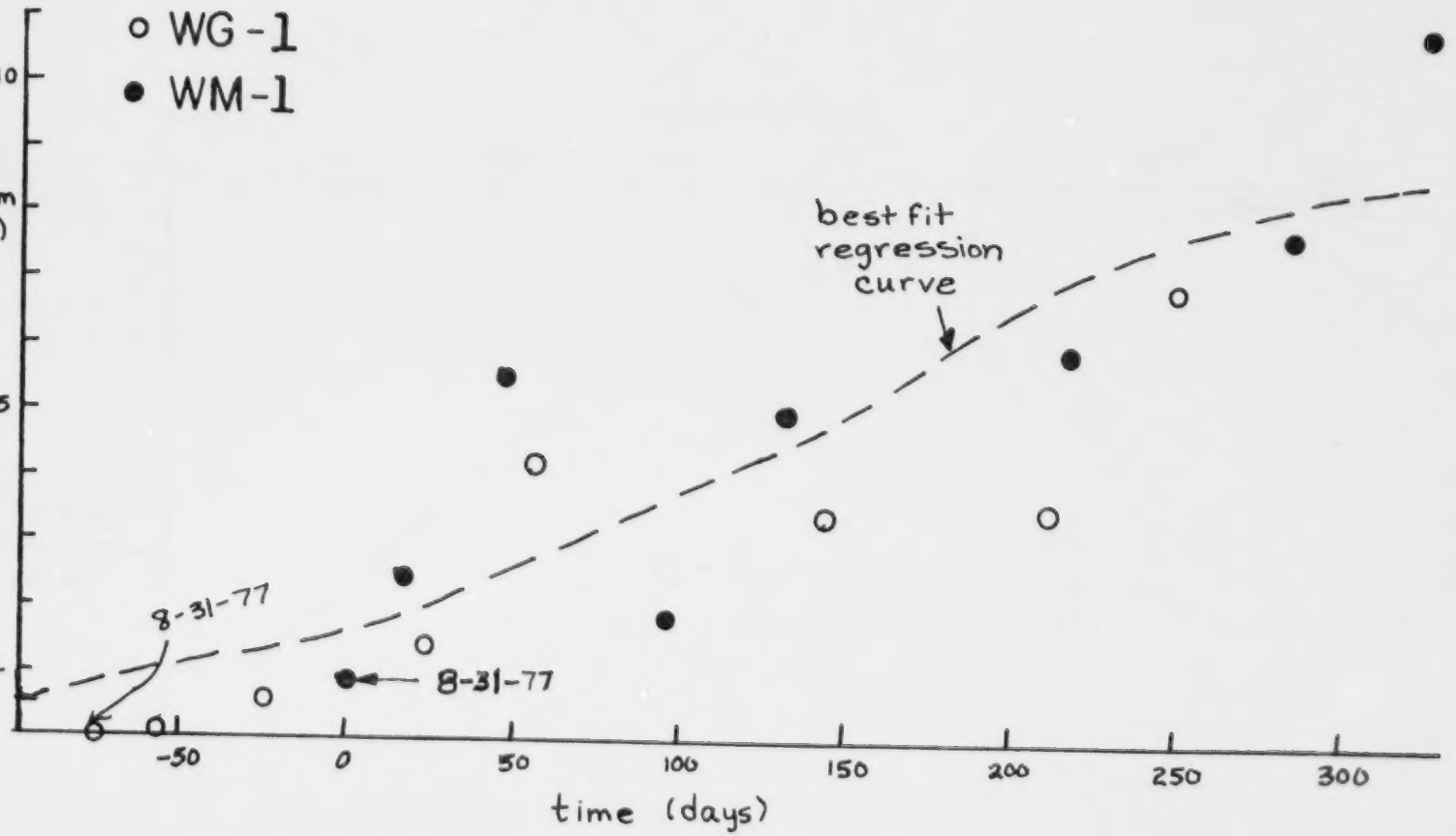


Fig. 9 Time History of Chromium in wells WM-1 and WG-1

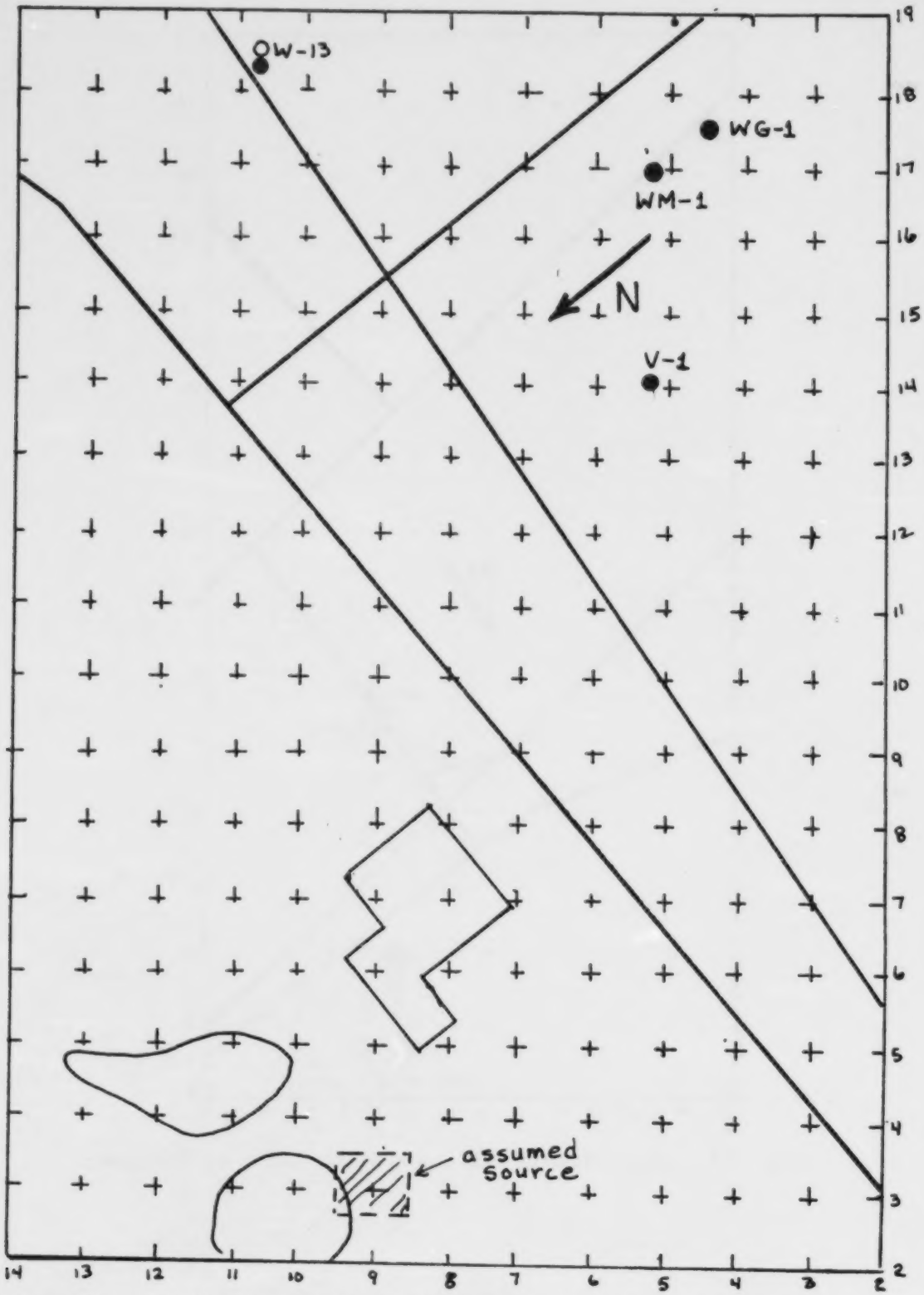


Fig. 10. Small Numerical Simulation Grid at Richland

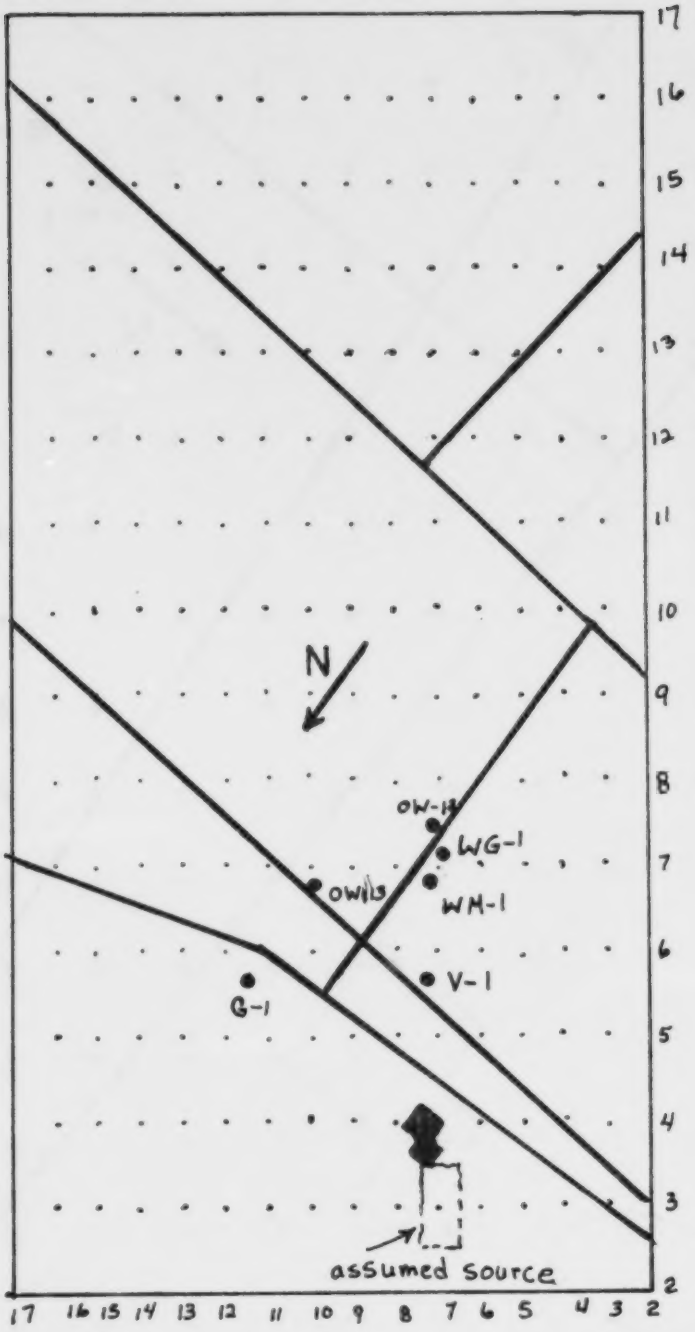


Fig. 11 Large Numerical Simulation Grid at Richland

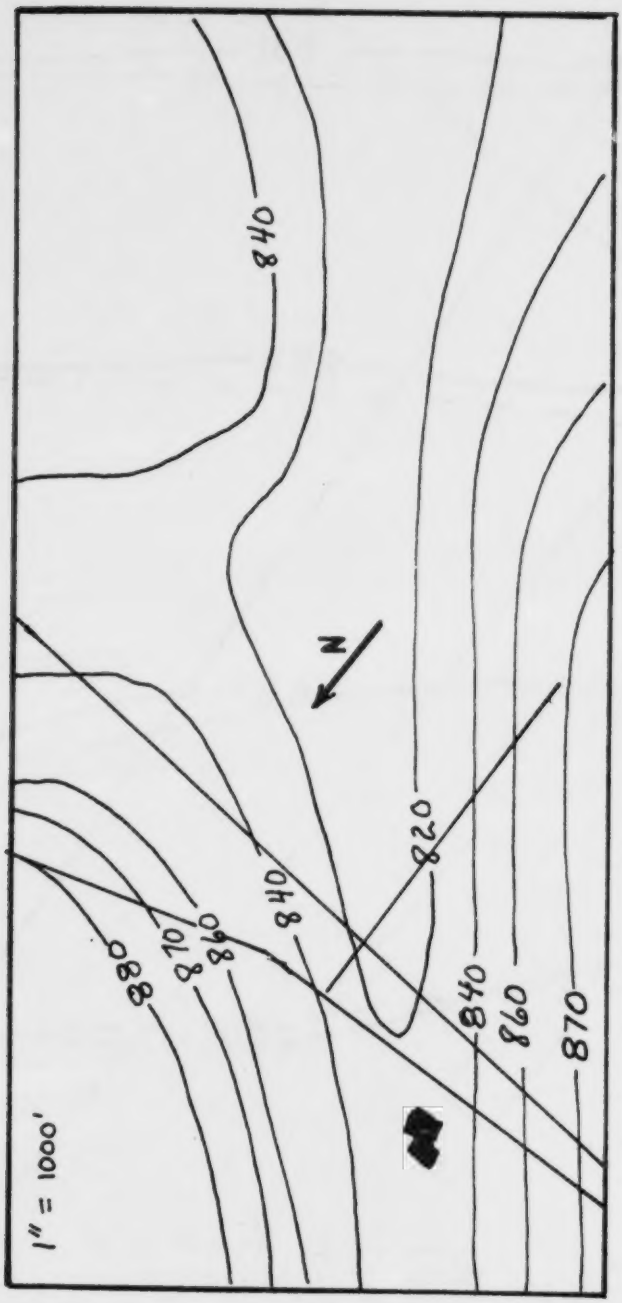


Fig. 12 Aquifer Bottom Elevations used in Numerical Simulation

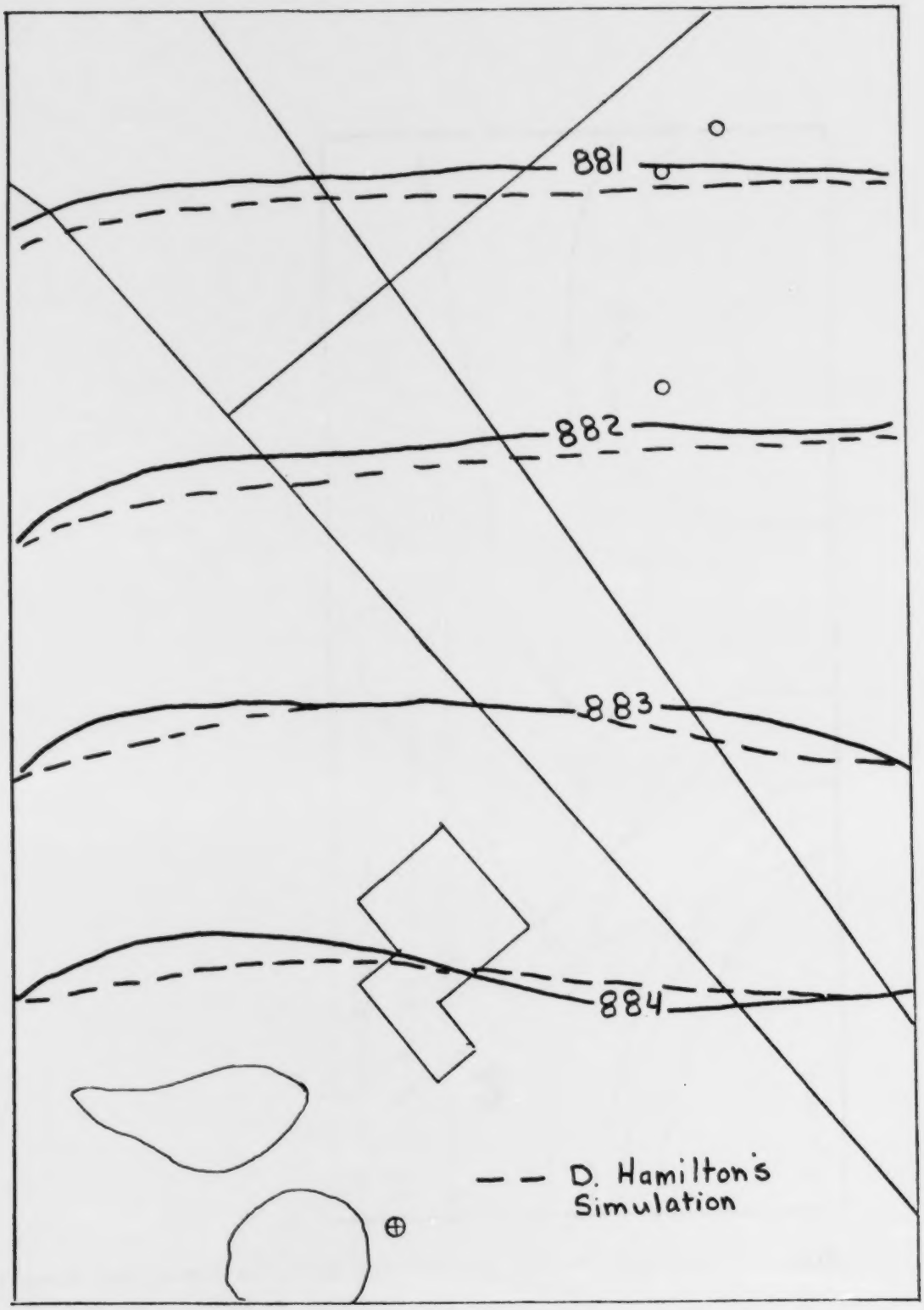


Fig. 13 Steady Water Table Elevations Computed with Small Grid

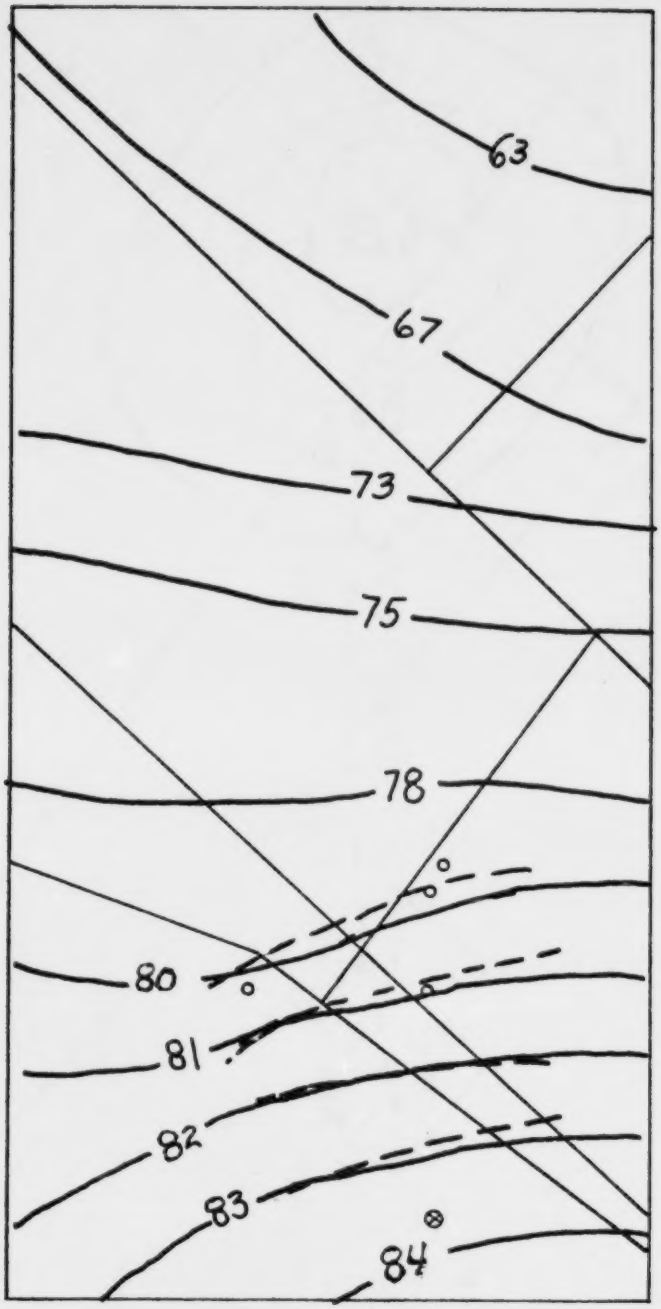


Fig. 14 Steady Water Table Elevations Computed with Large Grid

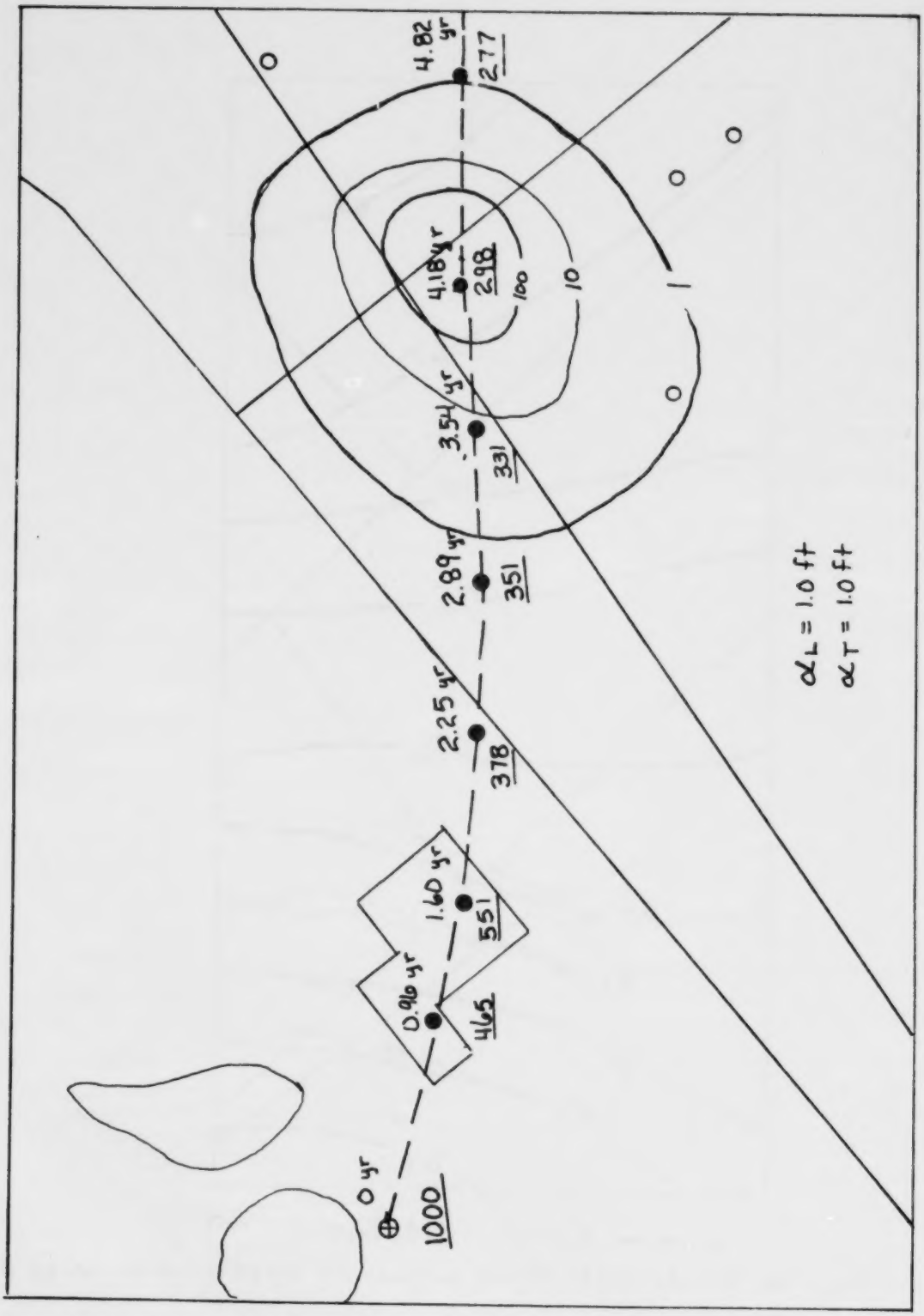


Fig. 15 Computed Plume Path and Profile at 4.18 years from small grid (arbitrary concentration units)

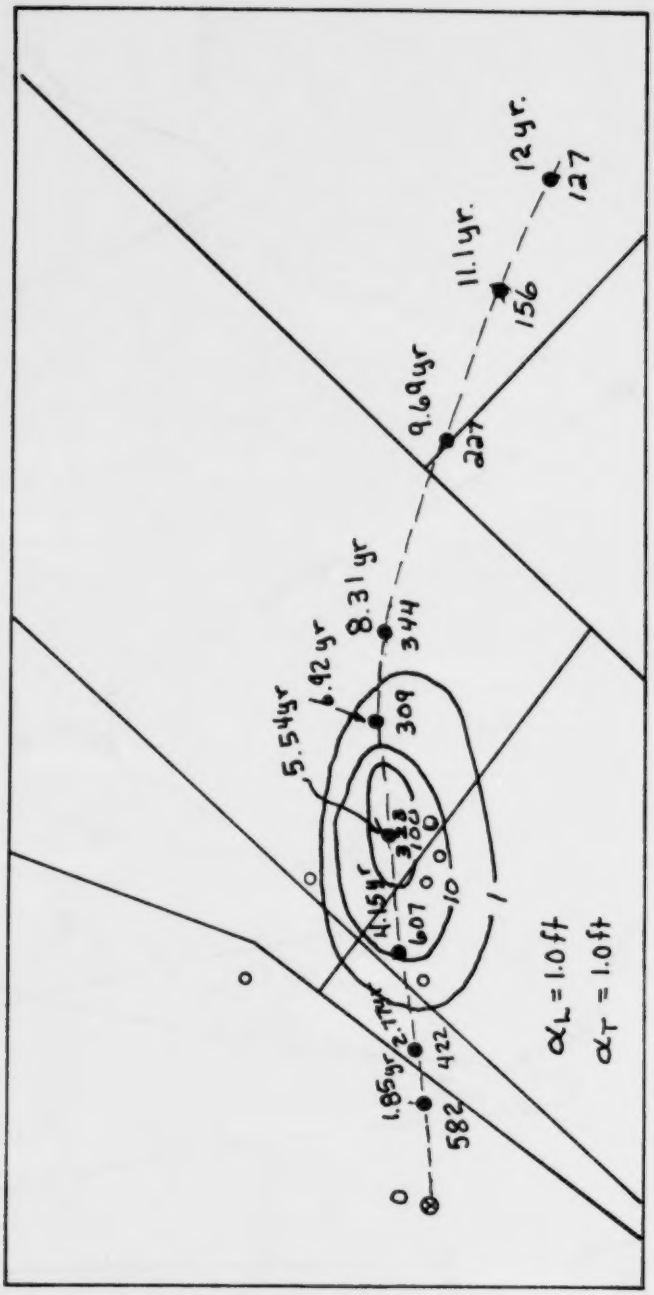


Fig. 16 Computed Plume Path and Profile at 5.54 years from large grid (arbitrary concentration units)

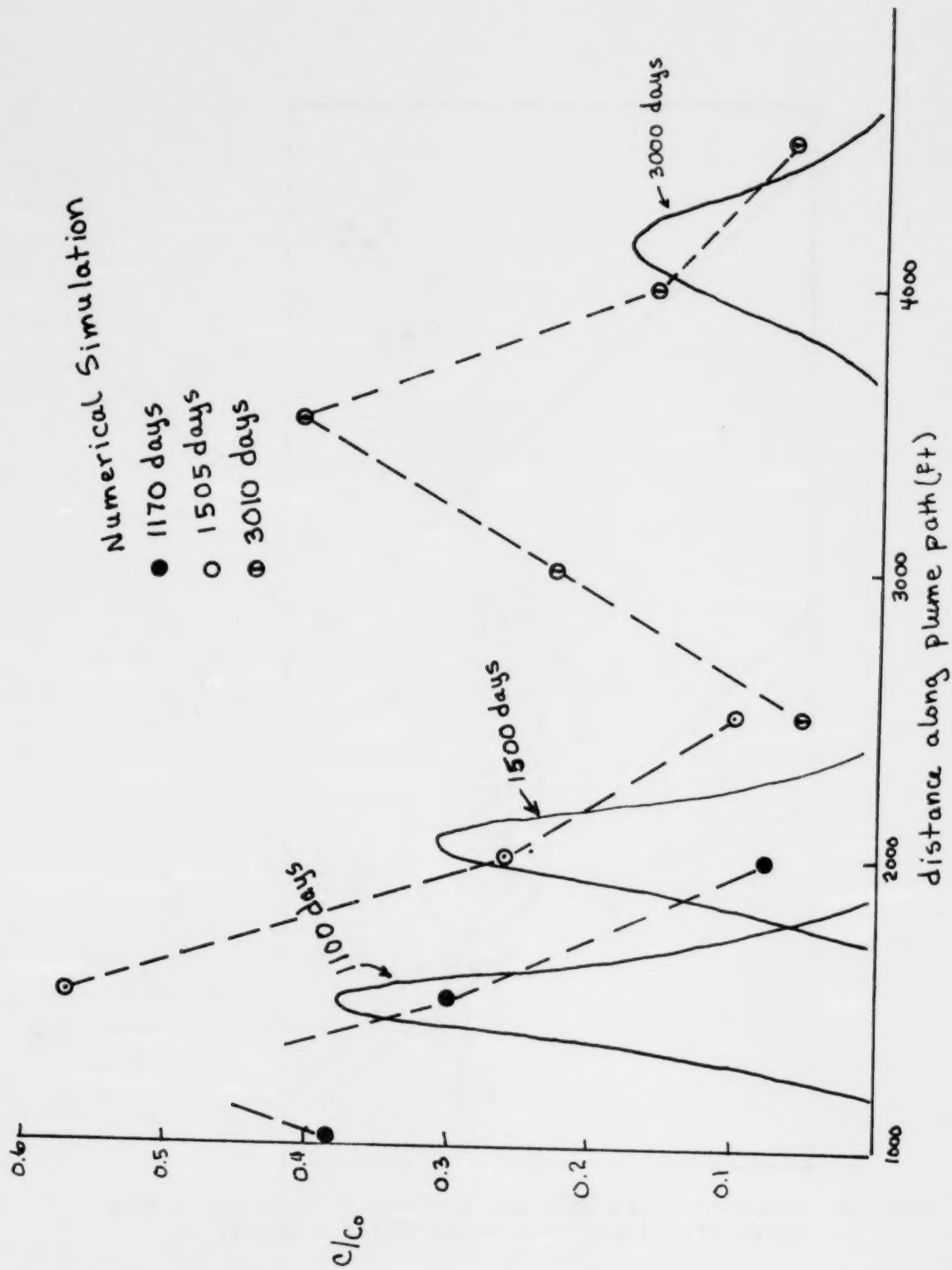


Fig. 17 Comparison of Longitudinal Profiles and Analytical Solutions

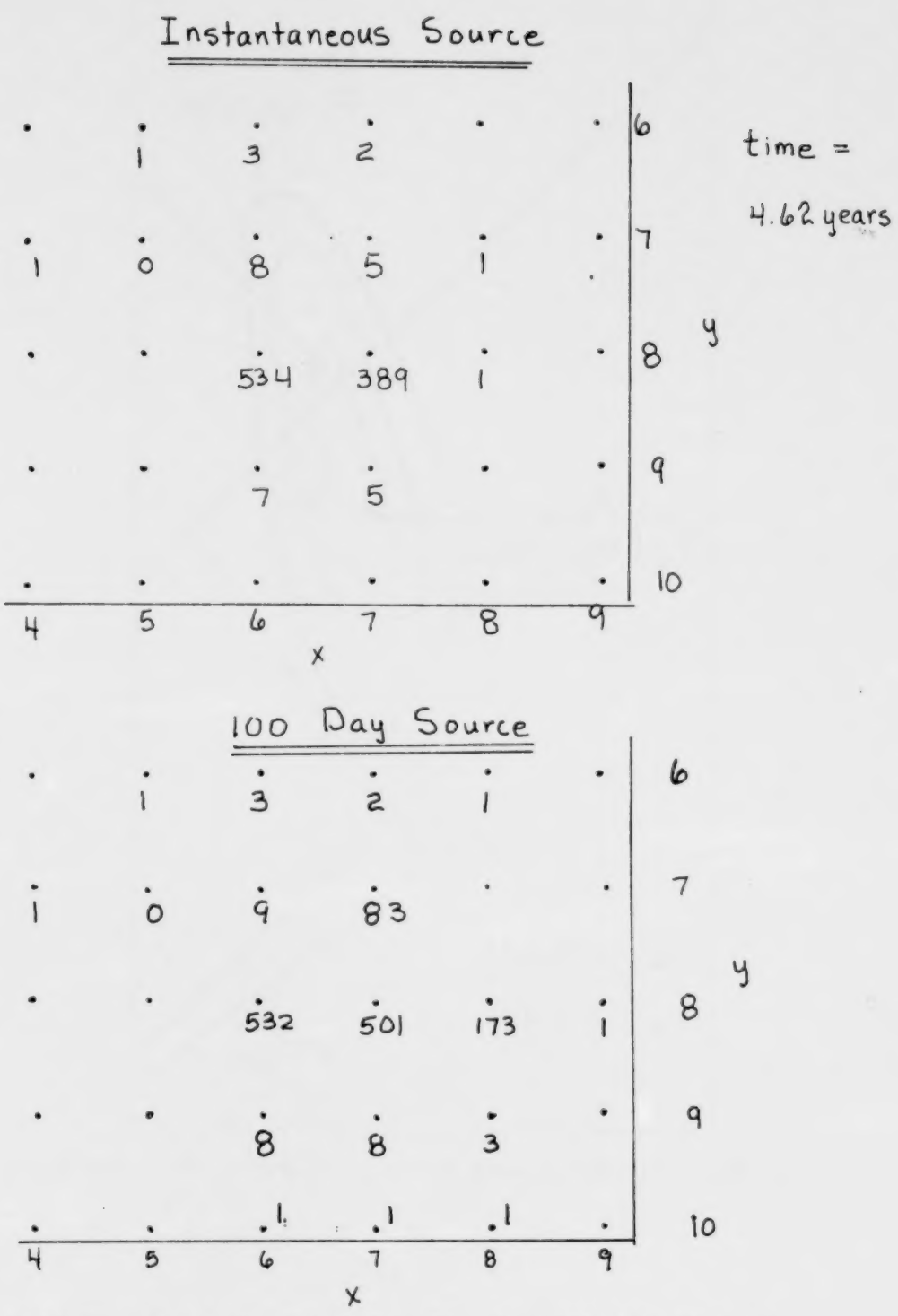


Fig. 18 Differences in Computed Results for 100 day Slug vs Instantaneous Source

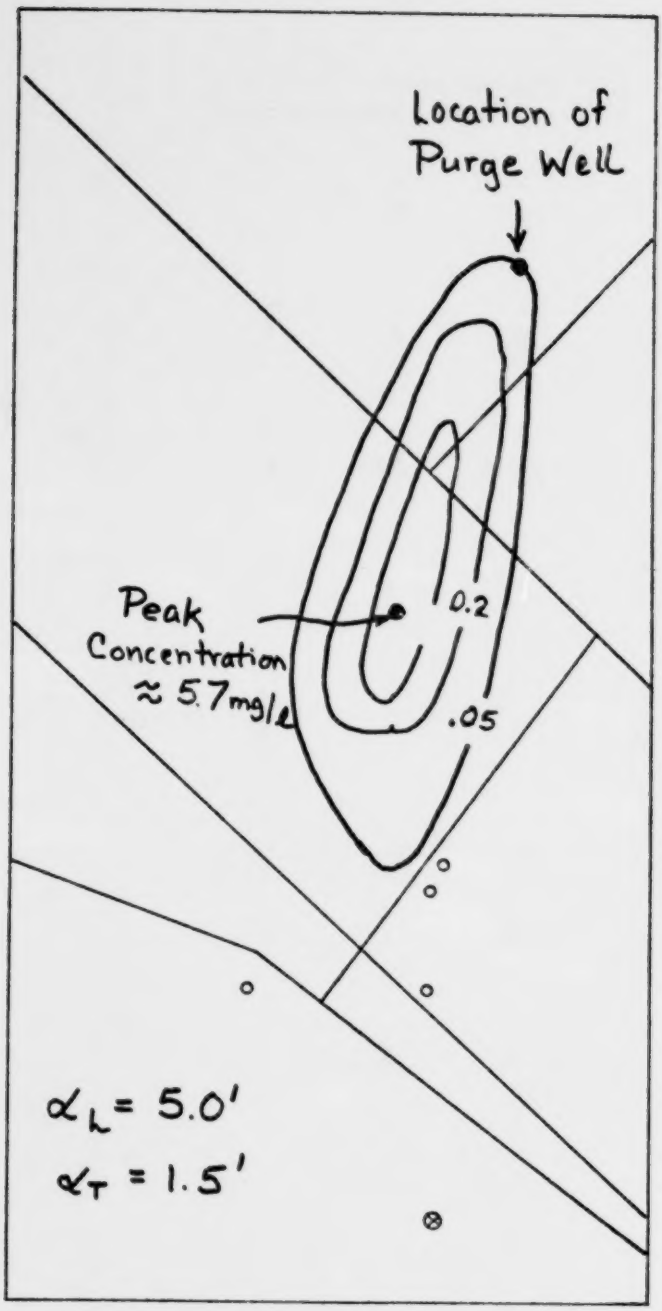


Fig. 19 Estimated Present (March, 1982) Chromium Location

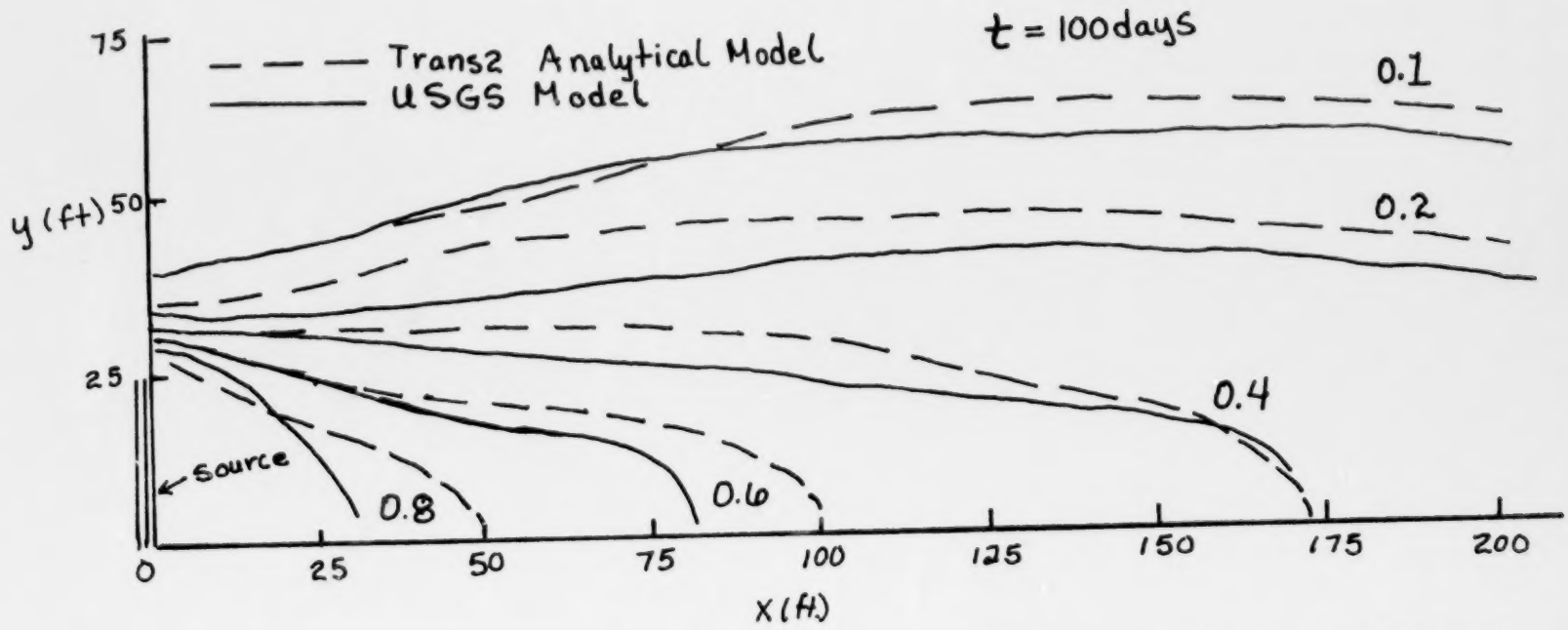


Fig. 20 Comparison of Analytical results with USGS model computations for an instantaneous strip source.

APPENDIX D

Finite Element Modeling of Contaminant Transport

by

D. C. Wiggert

GROUNDWATER MANAGEMENT STRATEGY FOR MICHIGAN

FINITE-ELEMENT MODELLING OF CONTAMINANT TRANSPORT

D. C. WIGGERT

March 1982

1. Introduction
2. Description of GEOFLOW
3. Model verification
4. Application of model to field study
5. Assessment of model
6. Conclusions and recommendations

1. Introduction

The study reported herein was initiated at the request of the Water Management Division of the Michigan Department of Natural Resources to assist in computer modeling aspects of groundwater contamination. Specifically, the finite element groundwater/transport model GEOFLOW, developed by D'Appolonia Consulting Engineers, Inc. is evaluated. The utility and accuracy of GEOFLOW is demonstrated by comparison with an analytical solution and by modeling an idealized flow situation.

A major effort has been expended upon the modeling of contaminant transport at the Production Plated Plastics site in Richland, Michigan. A calibration of the groundwater flow portion of the model was made by comparison with field data and with another finite element hydrodynamic model. In dealing with the prediction of transport, uncertainties increase due to vagueness surrounding the nature of the input loading, the estimates of the dispersion parameters, and inherent inaccuracies present in the algorithm. The latter, which consist of numerical oscillation and dispersion, may restrict the application of the model in obtaining precise quantitative predictions. However, a trained user may apply GEOFLOW to gain a qualitative understanding of the nature of contaminant transport. The model is adaptable to a regional aquifer system; however, it is important to maintain a sufficiently low numerical Peclet number to minimize numerical errors. Furthermore, it is recommended that sensitivity and accuracy studies be conducted as a part of any field study.

2. Description of GEOFLOW

The algorithm used in the present study is considered to be representative state-of-the-art finite element model for groundwater flow and contaminant transport. The computer code GEOFLOW was developed at D'Appolonia by Dr. Sirous Haji-Djafari as an outgrowth of earlier models developed at Michigan State University (6). Although it has been adapted for use in the hydrologic impact assessment of small-scale coal mining, it can be used to predict the variation in water quantity and quality of groundwater resources under a variety of conditions. The reader is referred to the user's manual (1) for detailed documentation. Features of the model are excerpted from that document and presented in the following.

In GEOFLOW the finite element method is used to discretize the governing partial differential equations. The program consists of two independent subprograms--the hydrodynamic model and the mass transport model. By utilizing appropriate input data such as transmissibility, storage coefficients, pumping rates, etc., the hydrodynamic model evaluates piezometric heads and velocity vectors. In turn the velocity vectors are employed by the mass transport model to compute the mass concentration distribution in the flow domain. Transient and steady-state solution of flow and of mass transport can be facilitated by the program.

The mathematical equations describing flow and mass transport through a confined, semi-confined, or unconfined aquifer in a two-dimensional horizontal plane, as well as their finite-element discretization, are described in a number of texts (2,3,4). Briefly, the domain of investigation is divided into a group of isoparametric elements. Employing the Galerkin-based finite element method, the mathematical relations are transformed to a system of first-order partial differential equations which are solved to yield piezometric heads and mass concentrations at nodes.

For most practical purposes, at relatively low concentrations it can be assumed that the mass concentration does not affect the velocity distribution (2); hence the solution of a dispersion problem is decomposed into two independent subproblems. First, the velocity distribution is determined throughout the flow domain. Second, that velocity distribution is substituted into the dispersion equation, which in turn is solved for the concentration distribution in the flow domain. Velocity vectors play a dominant role in the convective-dispersion equation. They appear in the convective term as well as the dispersion coefficient, hence realistic and accurate evaluation of the velocity components is important. In GEOFLOW, simultaneous solution of the velocity vectors from piezometric heads provides continuous velocities at each node in the flow domain.

It is known that the finite-element method will provide an accurate numerical solution of the hydrodynamic problem. However, the method applied to mass transport produces less accurate results. As noted by Pinder and Gray (4), the reason it is more difficult to obtain a numerical solution of transport than of flow is because the mass transport equation contains a convective as well as a dispersive term. The finite element discretization in the spatial domain, coupled with the time derivative approximation, produces an undulating propagation front of solute (termed undershoot/overshoot), as well as numerical dispersion, which tends to smear the front. This is especially problematical when convective transport dominates over diffusive transport.

Presently, procedures to partially minimize these effects represent the state-of-the-art (4). The phenomena have been observed in GEOFLOW and seem to be consistent with similar finite-element models. Recent literature (e.g., 5) reports improved solutions for one-dimensional mass transport

with employment of time-variable grid sizing. However, for two-dimensional problems such techniques apparently remain in developmental stages (5).

Two criteria can be utilized to assess the accuracy of a numerical model to simulate mass transport. One can define a numerical Peclet number

$$Pe = \frac{v\Delta\ell}{D_\ell} = \frac{\Delta\ell}{\alpha_\ell}$$

in which v is the fluid velocity, $\Delta\ell$ a representative grid length, D_ℓ is the dispersion coefficient in the ℓ-direction, and α_ℓ is the dispersivity in the ℓ-direction. The Peclet number can be interpreted to indicate the prominence of convection relative to dispersion in the mass transport phenomenon. The second term is the numerical Courant number

$$Co = \frac{v\Delta t}{\Delta\ell}$$

in which Δt is the fluid velocity. This parameter is indicative of the distance a trace element has traveled relative to the grid size.

In a strict sense these numbers are applicable only to one-dimensional flows and mass transport, but they can provide an approximate guideline for simulation of two-dimensional flows or mass transport. A frequently adopted procedure is to maintain Pe not much greater than unity, and to treat unity as an upper bound on Co (5). In regional aquifer situations, the Courant condition usually can be satisfied with no difficulty; however, it may be difficult to maintain low Pe numbers. Associated with high Pe is the undesirable aspect of numerical oscillation of concentration fronts.

3. Model Verification

Two tests were performed to assess the efficiency and accuracy of the transport portion of GEOFLOW. The first one simulated a one-dimensional flow field with two-dimensional transport, and the second simulated a two-dimensional flow field with two-dimensional transport. In both situations the flow field was time invariant.

The first example was configured to compare with the analytic solution of a finite source strip of pollutant in an infinite flow field, see Figure 1. The finite element grid is shown in Figure 2c. It consists of 171 elements and 200 nodes. A known velocity of 2 ft/day is prescribed in the positive x-direction. The known input is equivalent to a strip source of concentration 1.0 with a length 60 ft, symmetrical about the line y = 200 ft. The dispersion coefficients were 80 ft^2/day in the x-direction and 20^2ft /day in the y-direction.

Concentration contours are shown in Figure 2 for times of 10, 100 and 1000 days. Comparison with the analytical solution, shown also in Figure 2, appears to be excellent. The discrepancies, which are minor, occur close to the source at the boundaries (y = 0) for t = 1000 days. Because of the approximate nature of the finite element model, these differences are not unexpected and can be considered within reasonable and acceptable limits.

In an earlier analysis, a time step sensitivity was performed on a similar but smaller region. Figure 3 shows a comparison of simulations at t = 100 days for time steps of 1, 5, and 10 days. The predictions are very similar, and give evidence of the accuracy of the finite element discretization.

For the two examples shown in Figures 2 and 3, evaluation of Pe and Co in the x-direction (the principal flow direction) reveals that Pe does not

exceed 1.25 and that the maximum Co is 0.80. These are acceptable values, and the consistency in the predicted concentrations provide further evidence of accurate simulation.

In the second example, a two-dimensional steady flow field is generated as shown in Figure 4. Pumping of 100 m^3/day occurs at location B in a confined medium and a source of equal strength is situated at location A. A tracer with a relative concentration of 1.0 is injected continuously at the source and begins to propagate into the medium. Figure 5 shows concentration contours at 10, 20, and 50 days after injection. Note the symmetry about a diagonal line from the source to the sink. In this example, the longitudinal and transverse dispersivities are of equal magnitude (50 m).

Estimates of the numerical Peclet and Courant numbers can be made in either the x- or y-direction, with the result that Pe is approximately 0.10 and Co ranges approximately between 0.001 and 0.10. No analytic solution is available for comparison with the finite element prediction. The exercise serves to demonstrate the application of modeling mass transport in a two-dimensional flow field.

In summary, the two examples presented in this section reveal that accurate and practical numerical predictions of mass transport can be made with the finite element model. This is to be expected since the Pe and Co criteria have been satisfied. Further examples, including analytical verification, are provided in Reference 1.

4. Application of Model to Field Study

The major task of the present study was to model contaminant mass transport at the Production Plated Plastics site located in Richland, Michigan. The primary contaminant is chromium, and field data is available which gives evidence of a slug moving through regions of the aquifer. All hydrogeologic data used as input to the GEOFLOW model were obtained from Water Management Division personnel.

The layout of the finite elements progressed through three iterations, with each successive attempt improving either the hydrodynamic or the mass transport predictions. The four grid configurations are shown in Figures 6 to 9. The motivation for the first change was to more accurately model the regional flow patterns by expanding the aquifer boundaries and adjusting some of the field parameters. Consequently, satisfactory piezometric surfaces and velocities were attained. The second iteration was carried out to allow the finite elements to more closely conform to streamlines and equipotential lines, with the expectation that the mass transport would be more accurately modelled. The third iteration approximately quadrupled the number of nodes and elements; this was done to reduce the numerical Peclet number.

4.1 Flow Predictions. The following assumptions and approximations were made to facilitate the hydrodynamic solution:

1. The assumed bottom contours are shown in Figure 10. Each element is assigned an average bottom elevation.
2. The shaded region in Figure 10 represents a pinched-out area; it is modelled as a low permeability region, K = 1.2 ft/day.
3. The permeability in the aquifer is assumed constant, K = 120 ft/day.
4. Natural vertical recharge into the aquifer is assumed constant, N = 0.001826 ft/day.

5. Located at nodes A and B are point sinks, each pumping at the rate of 8950 ft^3/day.

6. At node C is located a point source, inputting 6600 ft^3/day; this represents the fluid input at the contaminant site.

7. At the aquifer boundaries, along line ab, Figure 10, designated nodes are assigned known piezometric heads; all other boundary locations are assumed to be regions of no flow.

The finite element grid in Figure 9 consists of 848 elements and 921 nodes. Smaller elements were located in the vicinity downstream of the contaminant site. The predicted piezometric contours are shown in Figure 11 and the steady-state discharge vectors at nodal points are given in Figure 12. As verification of the flow model accuracy, the predicted piezometric contours were compared with both available field data and the finite-element flow model AQUIFEM. The field data was obtained only in the vicinity of the contamination site and agreement was satisfactory. Nearly identical results were obtained with GEOFLOW and AQUIFEM over the entire modelled region. Note that steady flow conditions have been assumed, and these are subsequently utilized in the mass transport model.

4.2 Prediction of Mass Transport. The prediction of mass transport in the aquifer is based upon the following assumptions:

1. The flow field in the aquifer is time invariant.

2. The contaminant is injected into the aquifer as a point source, location C in Figure 10. The concentration is assigned an arbitrary value of 100000 units.

3. The duration of injection can be varied from twice the time increment up to continuous input.

4. The longitudinal dispersivity and transverse dispersivity are constant, media porosity is 0.25, and molecular diffusion is assumed zero.

5. The chromium species retardation factor is unity.

The modelled plume migration 1800, 3600, and 5400 days subsequent to injection is shown in Figure 13. Here the longitudinal and transverse dispersivities are 5 ft and 2 ft, respectively, the duration of injection is 100 days, and the time increment for the mass transport simulation is 50 days. The isoconcentration contours were plotted using SURFACE II (7). The leading edge of the slug movement is clearly discernable, and there is some evidence of dispersion taking place, but this may be due to numerical effects in addition to any physical phenomenon. The relative concentrations versus time at two locations downstream from the injection well are shown in Figure 14. The grid of Figure 9 was employed.

The regional grid sizing is placing a severe demand upon the accuracy of the model. In the longitudinal direction of flow, Pe ranges from 30 near the source to 120 in the lower reaches of the aquifer. The Co varies between 0.333 and 0.083, and hence poses no difficulty. Such large Peclet numbers are known to result in numerical oscillations as the front is propagating through the medium (5), and that phenomenon was observed in the present simulation. The necessary remedial measures for a fixed grid system with the given data would be to reduce the element sizes. See Section 5.2 for further discussion.

A sensitivity study was undertaken to assess the effects of perturbing the time step, dispersivities, and injection duration time. The grid configuration of Figure 7 was utilized. Table 1 shows the variation of the parameters in question. In the following discussion, the 50 day time step is considered to be the base value.

Run Number	Time Increment	Longitudinal/ Transverse Dispersivity	Slug Duration
	(day)	(ft)	(day)
1	25	5/2	200
2	50	5/2	200
3	100	5/2	200
4	100	50/20	200
5	50	5/2	100

Table 1

According to the Courant criterion, the time increment could be increased to perhaps 250 days without affecting the convection. Increasing the increment to 100 days caused slight decreases in peak concentrations and small variations in arrival times of peak concentrations at selected nodes; these differences were not considered significant. Decreasing the time step to 25 days resulted in negligible differences when compared with the 50 day increment output.

Increasing the dispersivity tended to attenuate the peak concentrations as well as decrease slightly the arrival time of the peak concentrations at selected nodes. Note with the 50/20 dispersivity values, the Peclet number range has decreased by an order of magnitude. Even so, numerical oscillations persisted and tended to obscure the delineation of the slug movement.

An injection duration of 100 days will input one-half the mass of pollutant compared to an injection period of 200 days. As the slug moved past a point approximately 1500 ft downstream of the pollution site, the corresponding reduction in peak concentrations was $\sim$0.65. Unfortunately, because of the inherent numerical errors associated with the grid configuration shown in Figure 7, the concentration peak of a slug as it migrated

downstream exhibited significantly more attenuation than would be expected from the actual physical dispersion and convection assumed to be present.

4.3 Interception of Plume. With the assistance of D'Appolonia personnel a purge well system was modelled with pumping to begin 3000 days subsequent to the injection of chromium at the PPP site. Twenty-two hours of CP time were required on the Prime 750 computer to simulate 5500 days of aquifer flow (it was necessary to predict both time variable flow and contaminant transport). Consequently, only one complete simulation has been completed, where a single 500 gpm purge well was located approximately at the leading edge of the plume. Unfortunately, the pumping rate was too extreme and resulted in dewatering the aquifer too rapidly, thereby failing to properly intercept and purge the plume.

When designing a purge well system, it is probably more important to assess the hydrodynamic response due to well placement than to attempt to model the subsequent contaminant migration. If the wells are properly located, the predicted flow patterns should reveal how successful the interception will be. In attempting to model the subsequent contaminant movement, the resulting numerical uncertainties can likely prevent one to make an accurate estimation of the residual contaminants present in the system.

Two possibly viable purge well systems have been selected and the resulting hydrodynamic solutions are shown in Figures 15 and 16. In Figure 15, two purge wells (F,G) are each pumping 150 gpm and in Figure 16, an additional third well (H) is pumping 100 gpm. The flow patterns indicate that with either of these two arrangements, a significant portion of the plume will be intercepted. Work is currently underway at D'Appolonia to optimize the purge well system and to predict the resulting migration of residual contaminants in the aquifer.

4.4 Conclusions from Case Study. The grid sizing of Figure 9 was used to model the plume movement shown in Figure 13. The discretization consists of 848 elements and 921 nodes. The computations were performed on the Prime 750 minicomputer at D'Appolonia headquarters in Pittsburgh. The large storage requirements for that grid size necessitated segmenting the program and using approximately 4 hours of CP time to model the plume migration. Most likely, one would not attempt any further refinement with respect to grid size for an aquifer region of such magnitude, since computer size limitations and costs would become prohibiting factors. When attempting to model both time variable flow and convection/dispersion the CP time and consequent computing costs increase dramatically.

Due to the large numerical Peclet numbers present in even the most refined simulation ($30 < Pe < 120$), the accuracy of the contaminant model is restricted. It is worthy to note that significant improvement was seen in the predictions when comparing the results using the grid in Figure 9 with the less refined configurations of Figures 6 to 8. Any further refinement with GEOFLOW would be achieved by delineating a more localized flow region, thereby effecting a smaller grid and accompanying Peclet number.

5. Assessment of GEOFLOW Model

5.1 Limitations. The primary constraint which will face a user of a fixed grid mass transport model such as GEOFLOW will be the necessity to employ a sufficiently large number of elements to minimize the numerical oscillation and dispersion. Realistically, it is not always possible to maintain the numerical Peclet number in the desired range, and as a result, some numerical errors will be present. This will be particularly significant for mass transport which is convection dominated (as is the situation for the PPP site study). Another way to decrease the Peclet number given a fixed grid size is to increase the dispersivity coefficients. This may not be desirable from a physical argument, but for increased numerical accuracy it may be a reasonable compromise.

Additional problems encountered in the present study were related to the shape of the finite element. The GEOFLOW mass transport model employs linear quadilateral isoparametric elements which consist of four nodes connected by straight lines. Undesirable elements are those which do not conform closely to a rectangular shape. If an element can maintain a nearly rectangular outline, then a solute will migrate through without having a residual buildup of concentration remain. Likewise, rectangular shaped elements will prevent large accumulations at edge nodes.

There was no difficulty in maintaining an appropriate numerical Courant number in the regional analysis. According to that criterion, the time step could have been increased approximately five times without affecting the modelled convection. The effect of increased time step upon the dispersion is not clear, and a sensitivity study should be considered in the future.

There is no numerical accounting of solute mass conservation in the model. Such a check should be made at selected times to insure the accuracy of the predictions. This is especially true of GEOFLOW inasmuch as predicted concentrations which drop below a selected arbitrary baseline value are equated to that value at the end of each time increment. As a result, it is possible that mass conservation errors may be accumulative, especially when Peclet numbers are high and significant numerical oscillation is present.

5.2 Applicability of Model. The use of GEOFLOW for the regional aquifer problem has demonstrated that convection-dominated flows may be difficult to model accurately with a fixed finite element model. It is important to keep the numerical Peclet number sufficiently low such that numerical oscillations do not obscure the movement of predicted fronts; D'Appolonia personnel have suggested that a practical upper limit to Pe is about five. An appropriate Pe can be maintained by employing smaller elements or by increasing the dispersivities. With the former one may be bound by computer size, but that could be partially overcome by modeling a more localized region rather than an entire aquifer. With the latter, greater dispersion will be predicted; whether this is tolerable must be assessed for each individual situation. It is useful to keep in mind the significant uncertainties associated with field estimates of dispersivities and allow a reasonable variation in the model to be tolerated.

It should be apparant that in contrast to the difficulties surrounding fixed-grid finite element modeling of mass transport, the hydrodynamic solution is relatively insensitive to such approximation. The GEOFLOW model provides an accurate and versatile flow solution, one representative of many available finite element models.

In the present field study, it would be appropriate to take the regional flow predictions and subsequently utilize them to delineate a more localized flow region wherein would be contained the plume movement. Such a procedure would allow a more refined grid to be placed in the region of interest, thereby possibly reducing Pe without increasing dispersivities beyond their uncertainty limits. It would be necessary to accurately match the regional flow and ensure that the plume movement is not affected by the artificial boundaries. This approach may be the most rational one to pursue for regional mass transport problems.

Alternate flow and mass transport models are available which utilize characteristic methods (7) or combine characteristic and random walk concepts (8). These may be more desirable than fixed-grid finite element formulations when the mass transport is convection dominated.

5.3 Conclusions and Recommendations. It has been shown that GEOFLOW provides an accurate prediction of aquifer flows. In addition, favorable predictions of mass transport were provided for idealized flow situations in which approximate numerical stability and accuracy criteria were maintained. On the other hand, some difficulties were encountered when attempting to model convection dominated mass transport on a regional scale. This was due to the numerical Peclet number being too high. If one is to use a fixed-grid finite element model such as GEOFLOW, then it is necessary to employ a sufficiently small grid sizing to eliminate the undesirable numerical oscillation.

In the present study, the regional aquifer system was divided into a maximum of 848 elements. Additional accuracy could be obtained by estimating the plume convection from a regional flow analysis and subsequently

delineating a localized region for mass transport prediction including dispersion as well as convection. Such a procedure is recommended if further application of GEOFLOW to the present regional system is desired.

Acknowledgements

Appreciation is extended to S. Haji-Djafari and T. H. Wells of D'Appolonia Consulting Engineers, Inc., for providing their expertise and assistance during the late stages of modeling the regional mass transport. Substantial computer time was donated by D'Appolonia. During the course of the study, D. A. Hamilton assisted in interpreting the numerical results and participated in useful discussions.

References

1. "Groundwater Flow Model GEOFLOW," User's Manual, D'Appolonia Consulting Engineers, Inc., Pittsburgh, Pa., December, 1980.

2. Bear, J., Hydraulics of Groundwater, McGraw-Hill, Inc., 1979.

3. Freeze, R. A., and Cherry, J. A., Groundwater, Prentice-Hall, Inc., 1979.

4. Pinder, G. F., and Gray, W. G., Finite Element Simulation in Surface and Subsurface Hydrology, Academic Press, 1977.

5. O'Neill, K., "Highly Efficient, Oscillation Free Solution of the Transport Equation Over Long Times and Large Spaces," Water Resources Research, Vol. 17, No. 6, pp. 1665-1675, December 1981.

6. Haji-Djafari, S., "Two-Dimensional Finite Element Analysis of Transient Flow and Tracer Movement in Confined and Phreatic Aquifers," Ph.D. Dissertation, Michigan State University, 1976.

7. Sampson, R. J., "Surface II Graphics System", Computer Services Section, Kansas Geological Survey, Lawrence, Kansas (1978).

Figures

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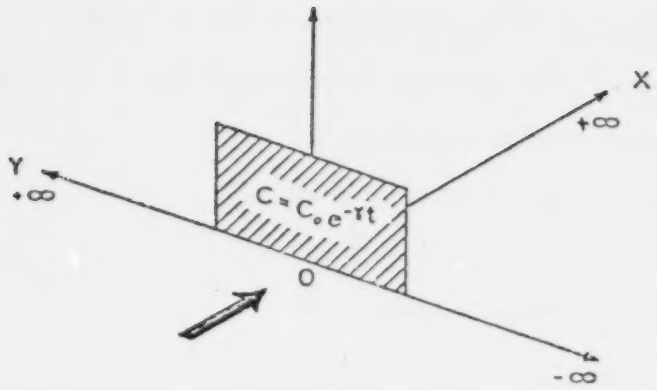
TWO-DIMENSIONAL INFINITE GROUND WATER MODEL



STRIP SOURCE

TWO-DIMENSIONAL MASS TRANSPORT EQUATION

(STRIP SOURCE — Infinite Width)

$$\frac{\partial C}{\partial t} + V_x \frac{\partial C}{\partial X} + V_y \frac{\partial C}{\partial Y} = D_x \frac{\partial^2 C}{\partial X^2} + D_y \frac{\partial^2 C}{\partial Y^2} - KC$$

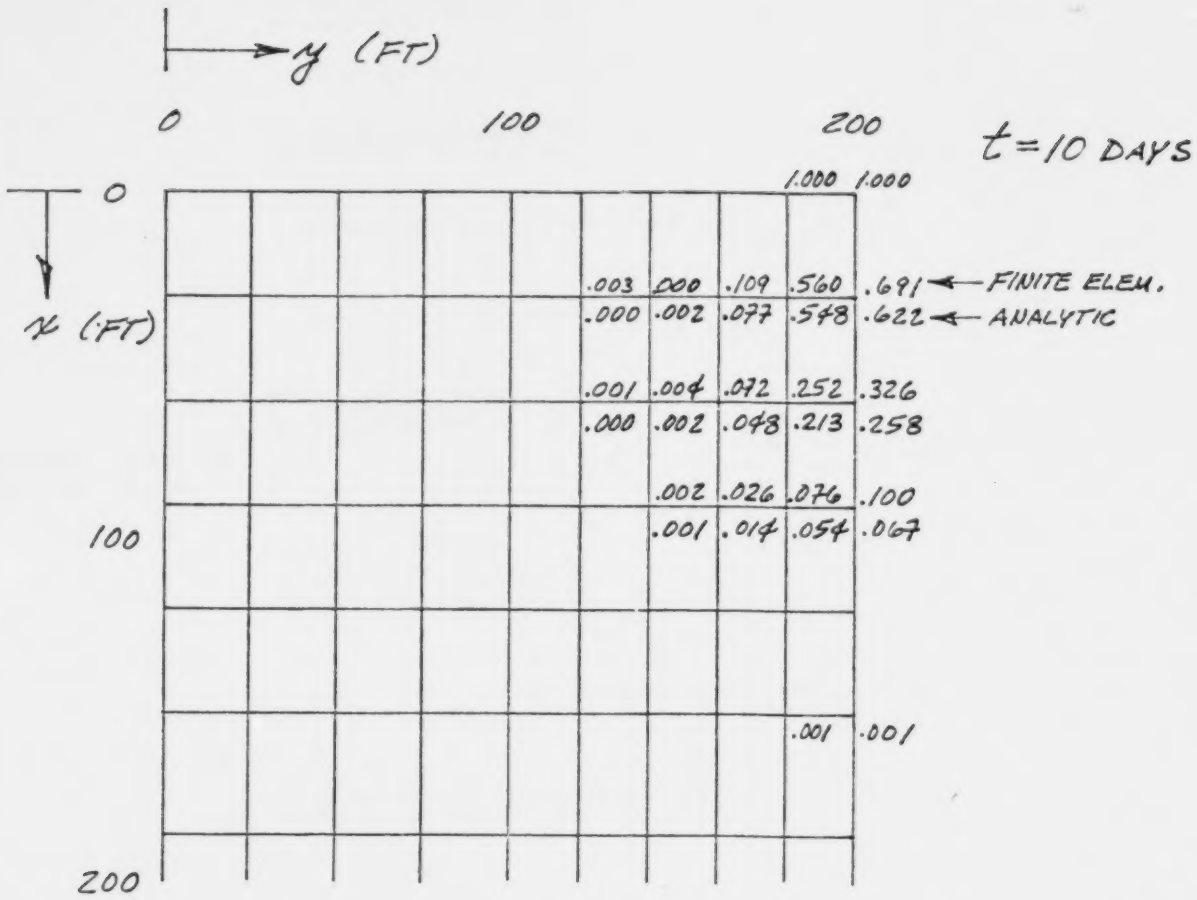
$C = C_0 e^{-\gamma t}$	$X = 0$	$Y_1 \leq Y \leq Y_2$
$C = 0$	$X = 0$	all other Y
$\frac{\partial C}{\partial Y} \longrightarrow 0$	$Y \longrightarrow \pm\infty$	
$\frac{\partial C}{\partial X} \longrightarrow 0$	$X \longrightarrow +\infty$	
$C = 0$	$t = 0$	

ANALYTICAL SOLUTION

$$C(X,Y,t) = \frac{C_0 X}{4\sqrt{\pi D_x}} e^{\left(\frac{V_x X}{2D_x} - \gamma t\right)} \cdot \int_{\tau=0}^{t} \frac{e^{-\left(K - \gamma + \frac{V_x^2}{4D_x}\right)\tau - \frac{X^2}{4D_x\tau}}}{\tau^{3/2}}$$

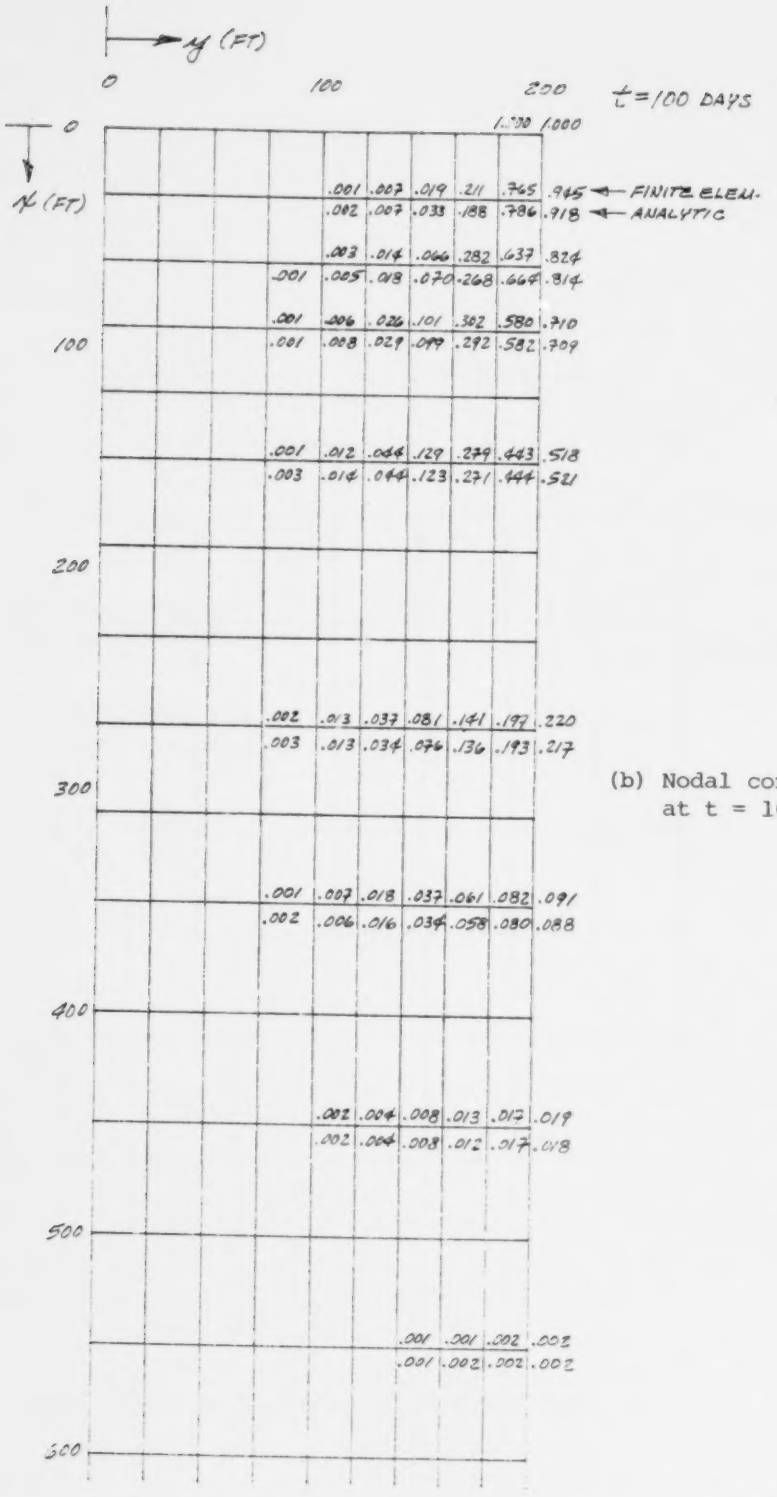
$$\cdot \left\{ - \operatorname{erfc}\left(\frac{(Y_2 - Y)}{2\sqrt{D_y \tau}} + \frac{V_y}{2}\sqrt{\frac{\tau}{D_y}}\right) + \operatorname{erfc}\left(\frac{Y_1 - Y}{2\sqrt{D_y \tau}} + \frac{V_y}{2}\sqrt{\frac{\tau}{D_y}}\right)\right\} d\tau$$

Fig. 1 Analytical Model



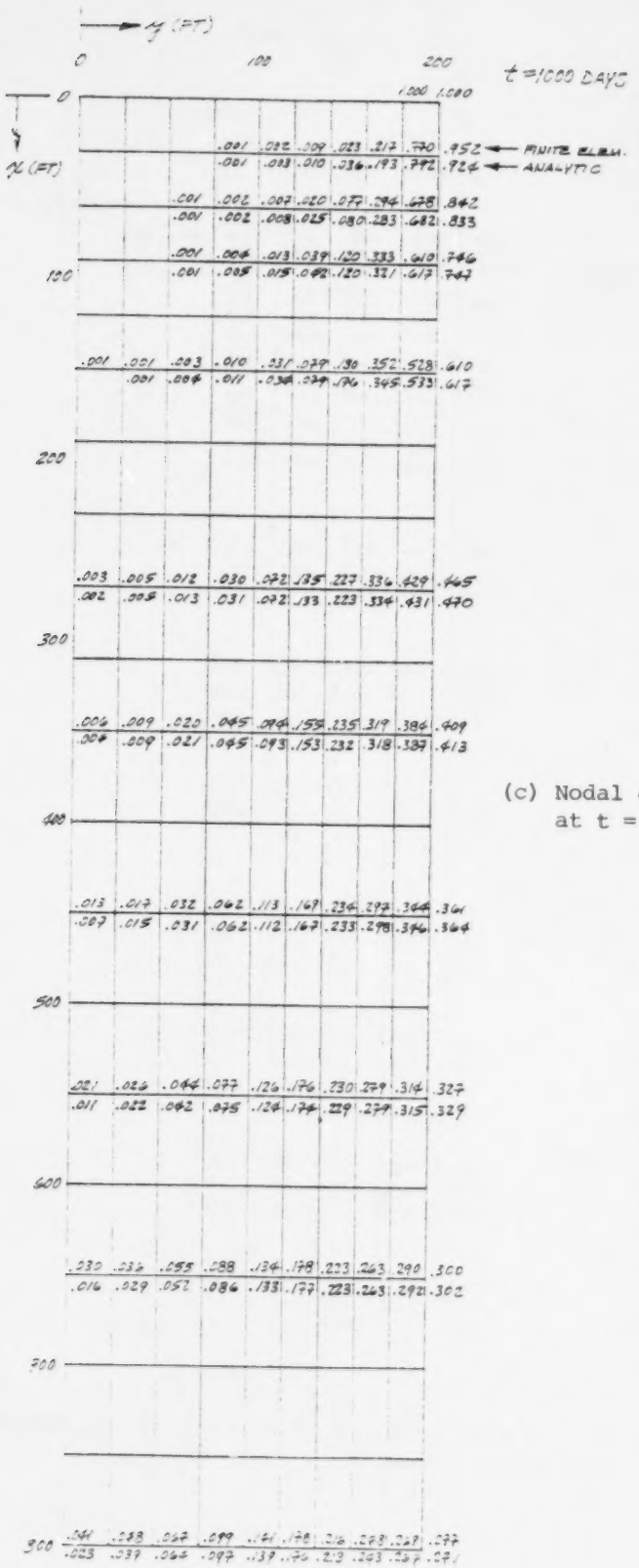
(a) Nodal concentrations at t = 10 days

Fig. 2 Finite element model of strip source: comparison with analytical model



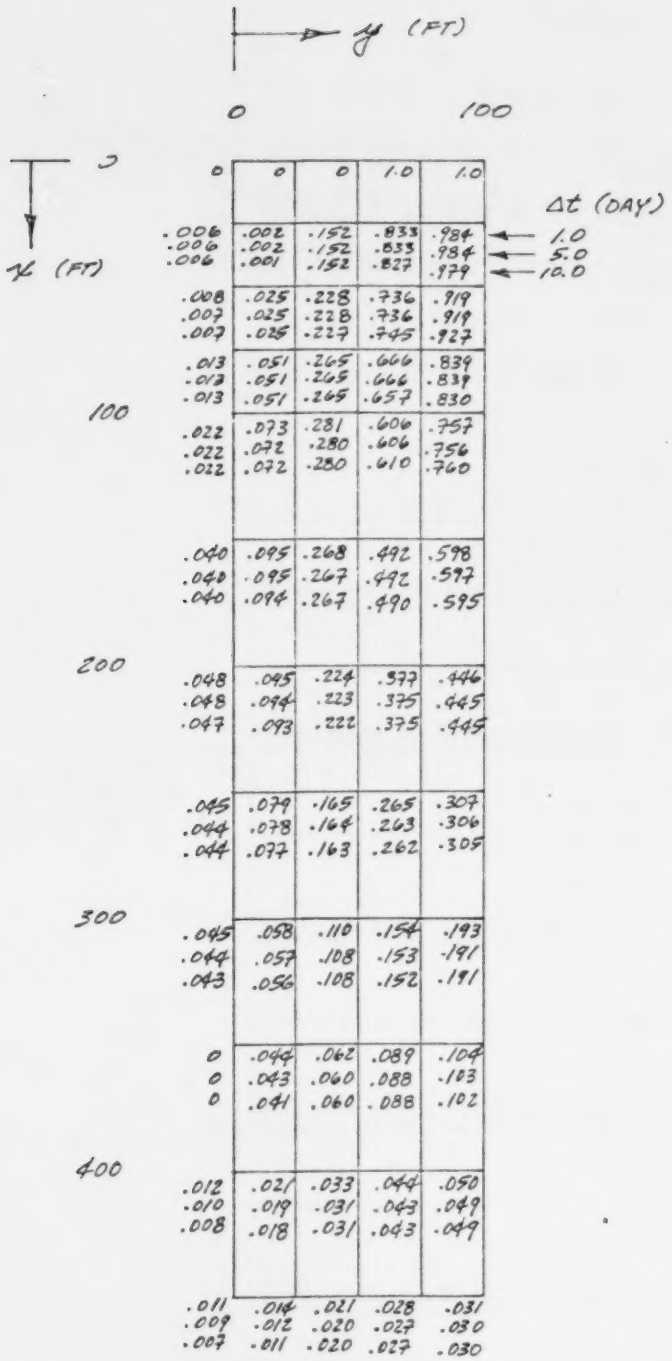
(b) Nodal concentrations at t = 100 days

Fig. 2 (continued)



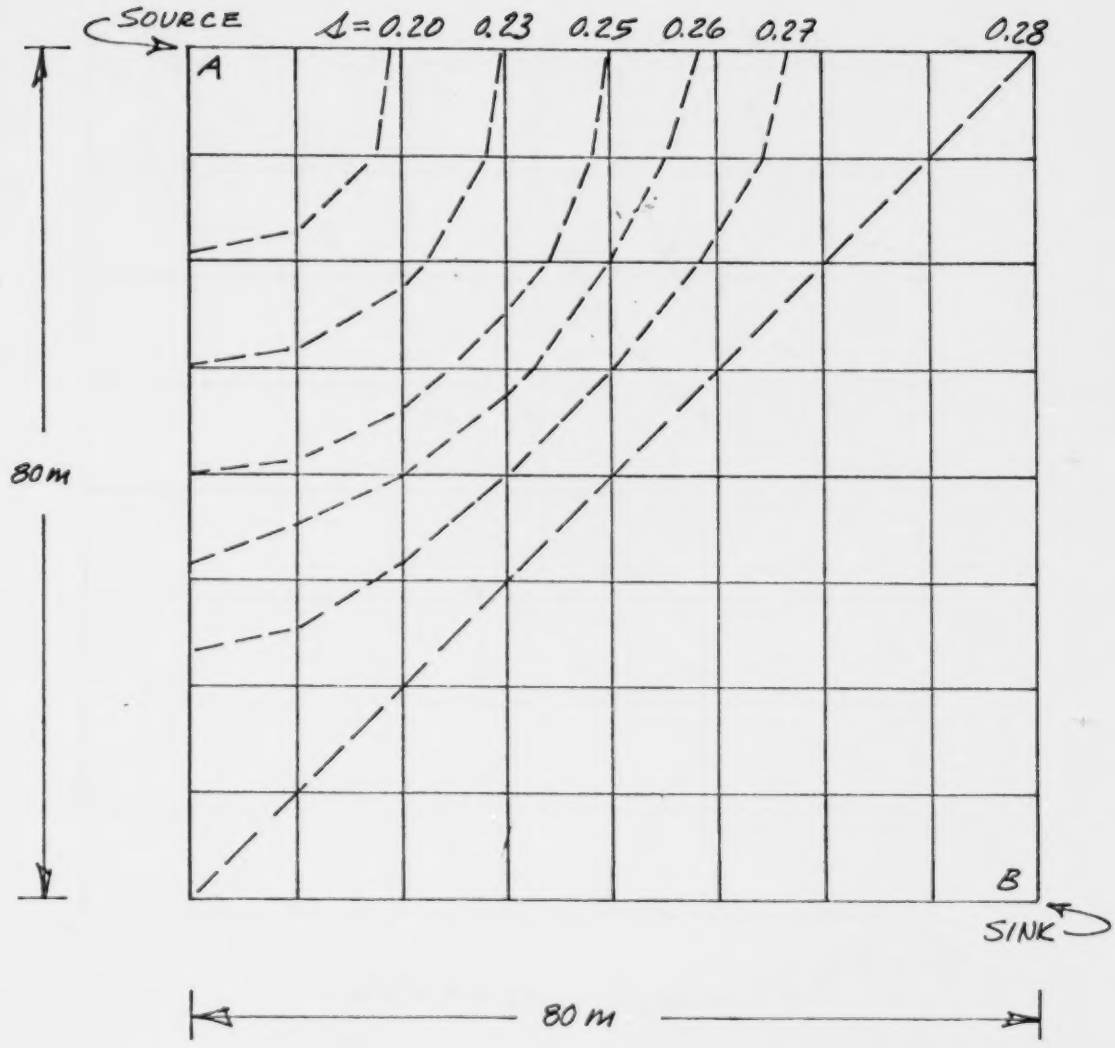
(c) Nodal concentrations at t = 1000 days

Fig. 2 (continued)



x (FT)	y = 0	y = 0	y = 1.0	y = 1.0	Δt (DAY)
.006	.002	.152	.833	.984	← 1.0
.006	.002	.152	.833	.984	← 5.0
.006	.001	.152	.827	.979	← 10.0
.008	.025	.228	.736	.919	
.007	.025	.228	.736	.919	
.007	.025	.227	.745	.927	
.013	.051	.265	.666	.839	
.013	.051	.265	.666	.839	
.013	.051	.265	.657	.830	
100					
.022	.073	.281	.606	.757	
.022	.072	.280	.606	.756	
.022	.072	.280	.610	.760	
.040	.095	.268	.492	.598	
.040	.095	.267	.492	.597	
.040	.094	.267	.490	.595	
200					
.048	.045	.224	.377	.446	
.048	.094	.223	.375	.445	
.047	.093	.222	.375	.445	
.045	.079	.165	.265	.307	
.044	.078	.164	.263	.306	
.044	.077	.163	.262	.305	
300					
.045	.058	.110	.154	.193	
.044	.057	.108	.153	.191	
.043	.056	.108	.152	.191	
0	.044	.062	.089	.104	
0	.043	.060	.088	.103	
0	.041	.060	.088	.102	
400					
.012	.021	.033	.044	.050	
.010	.019	.031	.043	.049	
.008	.018	.031	.043	.049	
.011	.014	.021	.028	.031	
.009	.012	.020	.027	.030	
.007	.011	.020	.027	.030	

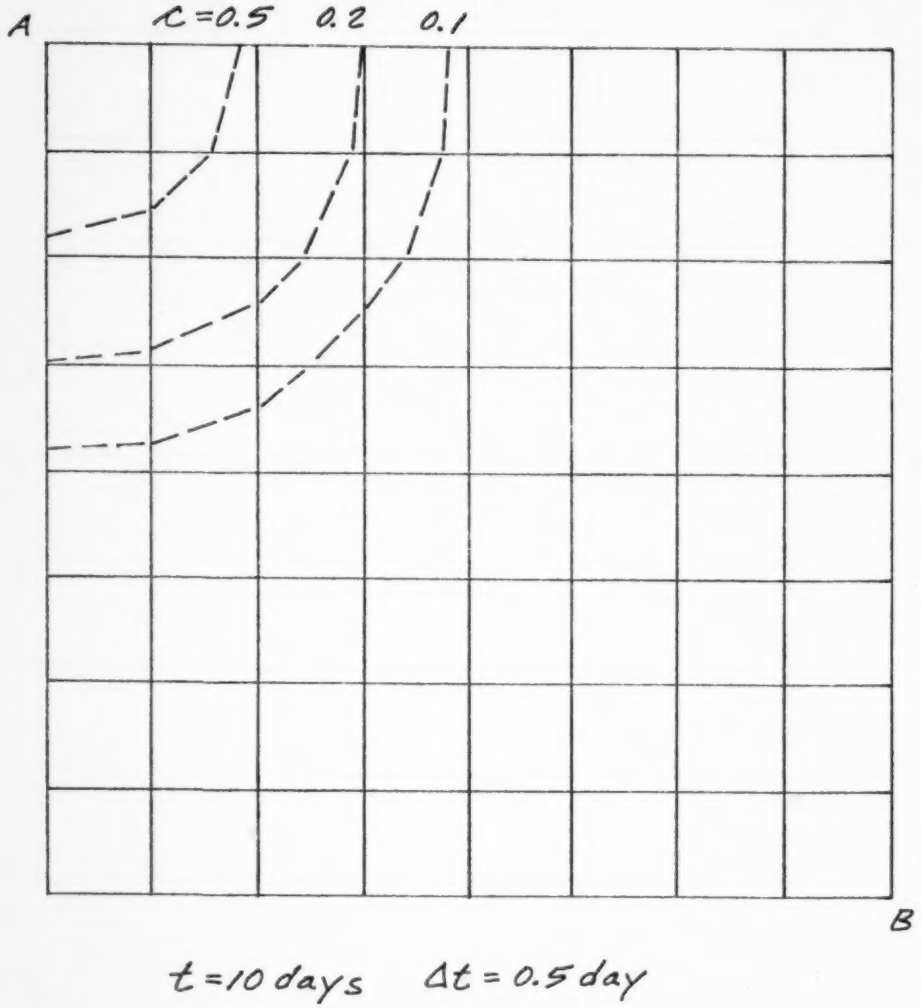
Fig. 3 Finite element model of strip source: comparison of time increment variation



$T_{11} = T_{22} = 900\ m^2/day$ $\quad n_e = 0.25$

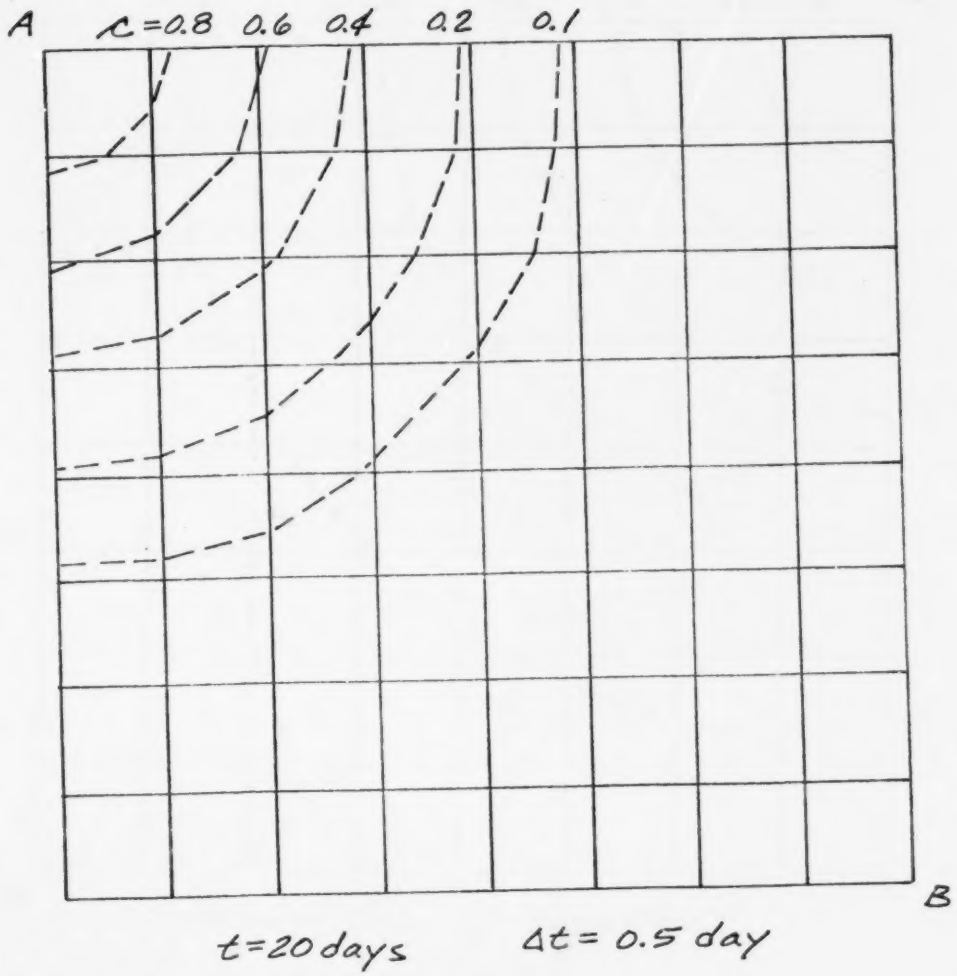
$\alpha_L = \alpha_T = 50\ m$ $\quad P = 100\ m^3/day$

Fig. 4 Finite element model of two-dimensional flow field



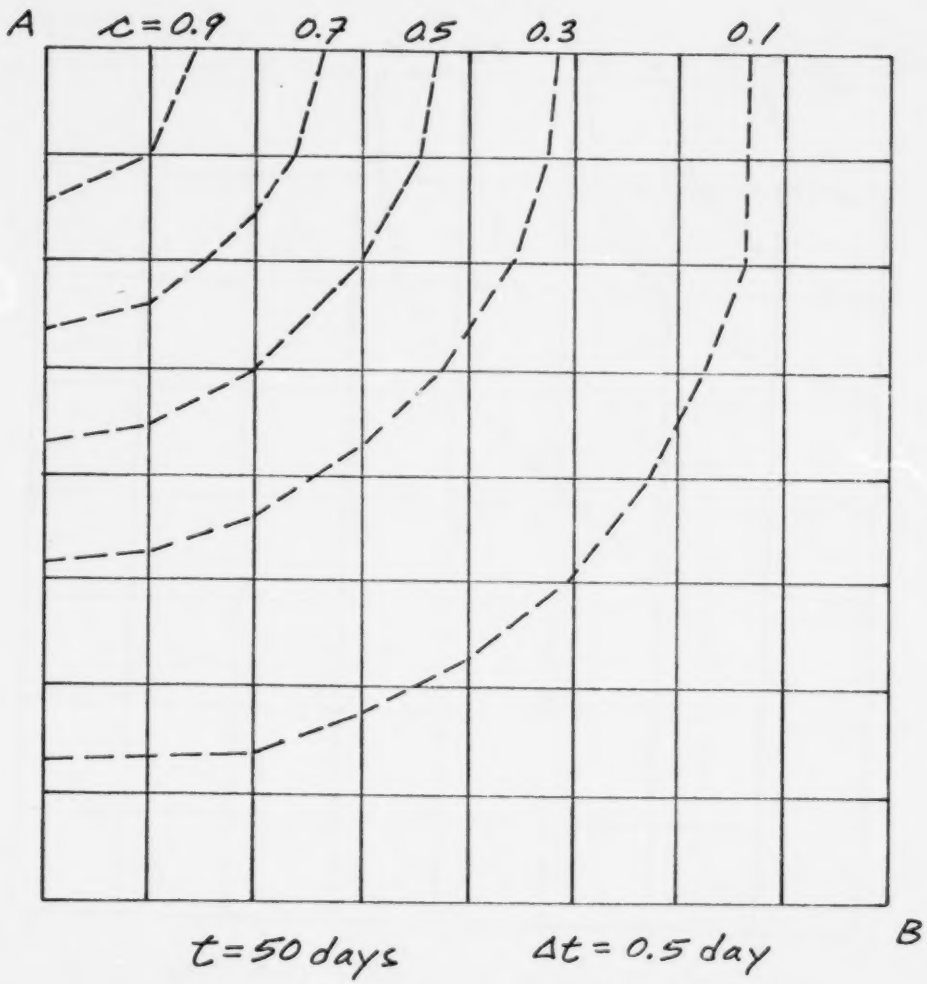
(a) Concentration contours at t = 10 days

Fig. 5 Predictions of mass transport in two-dimensional flow field



(b) Concentration contours at t = 20 days

Fig. 5 (continued)



(c) Concentration contours at t = 50 days

Fig. 5 (continued)

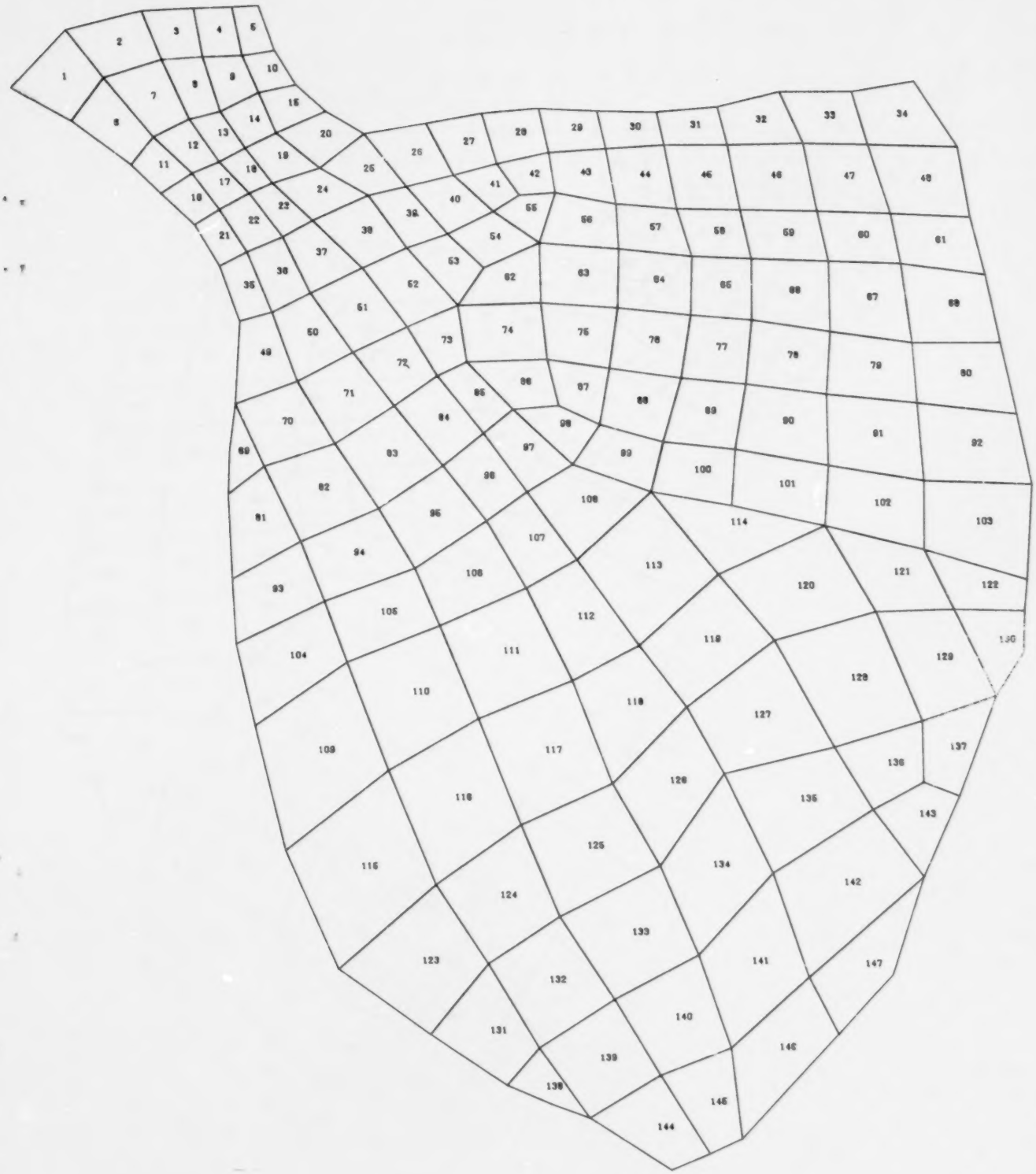


Fig. 6 First regional finite element grid

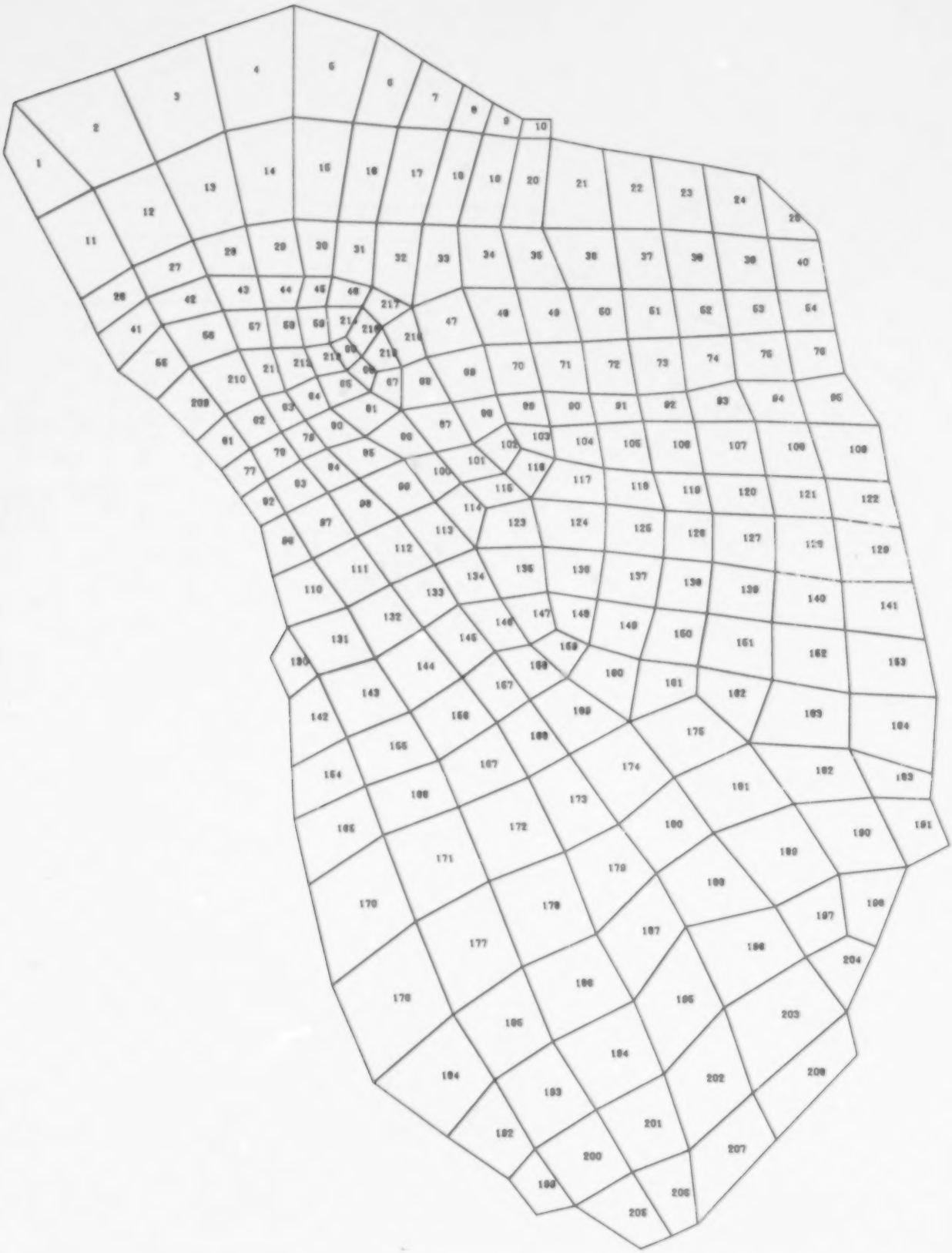


Fig. 7 Second regional finite element grid

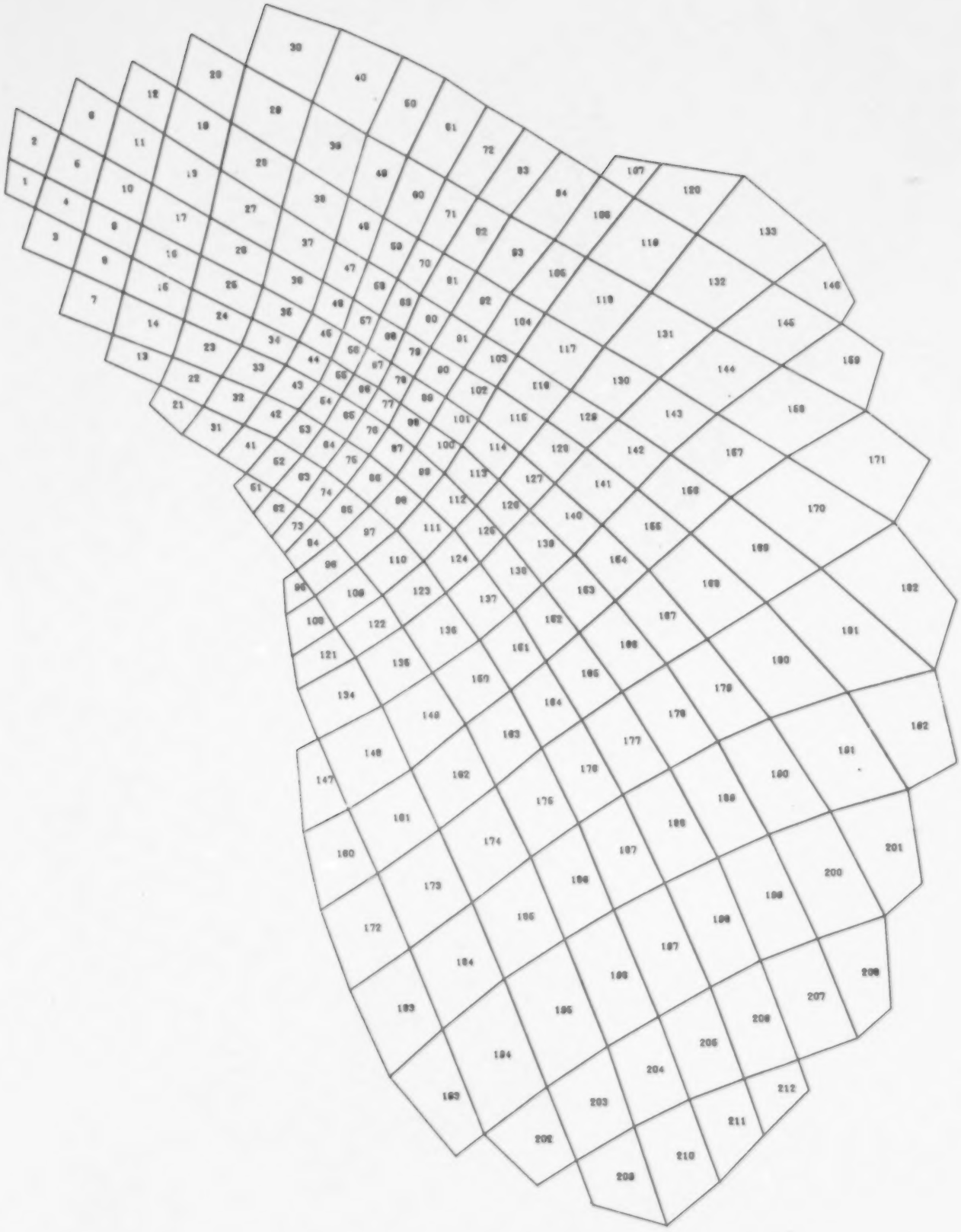


Fig. 8 Third regional finite element grid

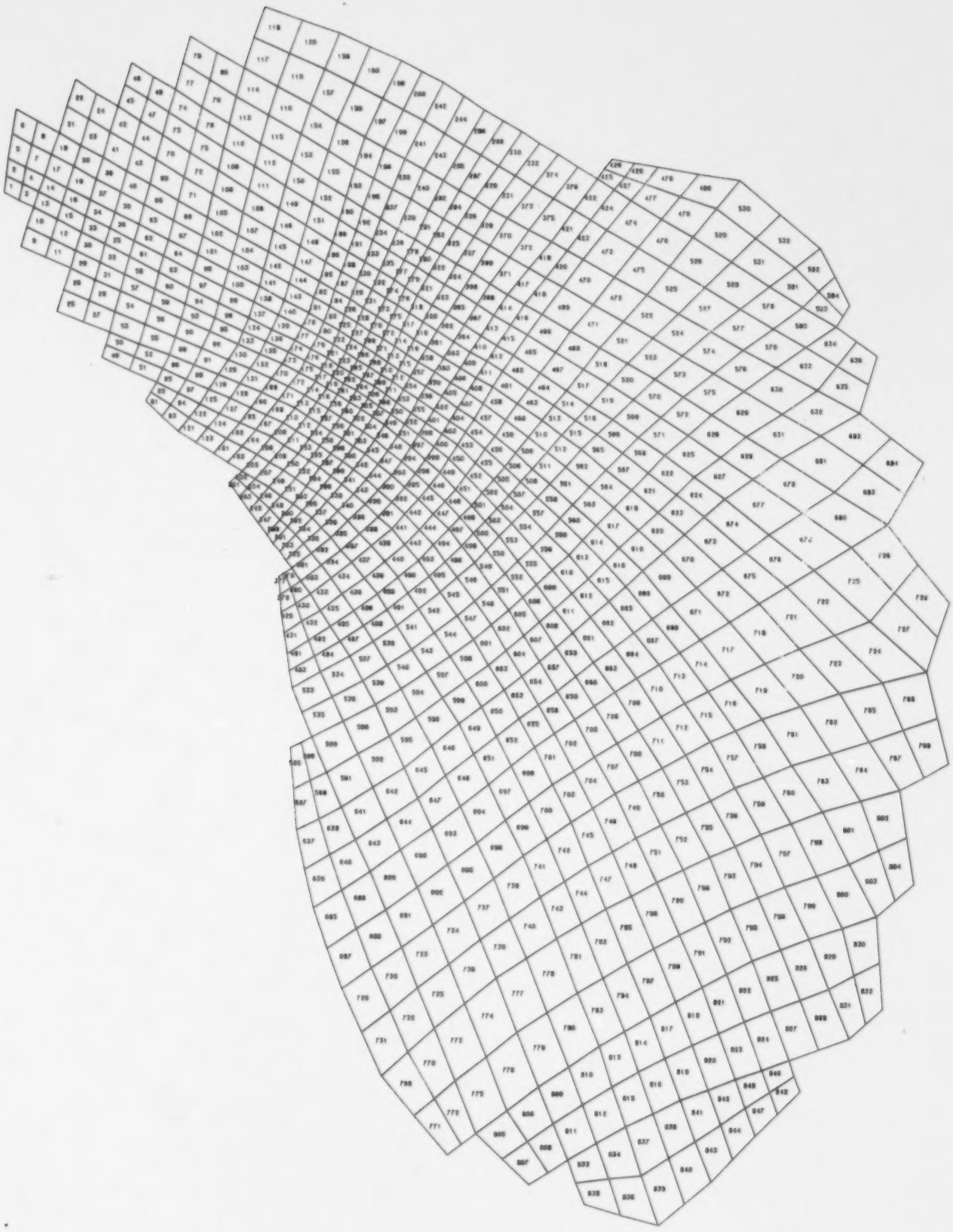


Fig. 9 Fourth regional finite element grid

Fig. 10 Elevation contours of aquifer bottom

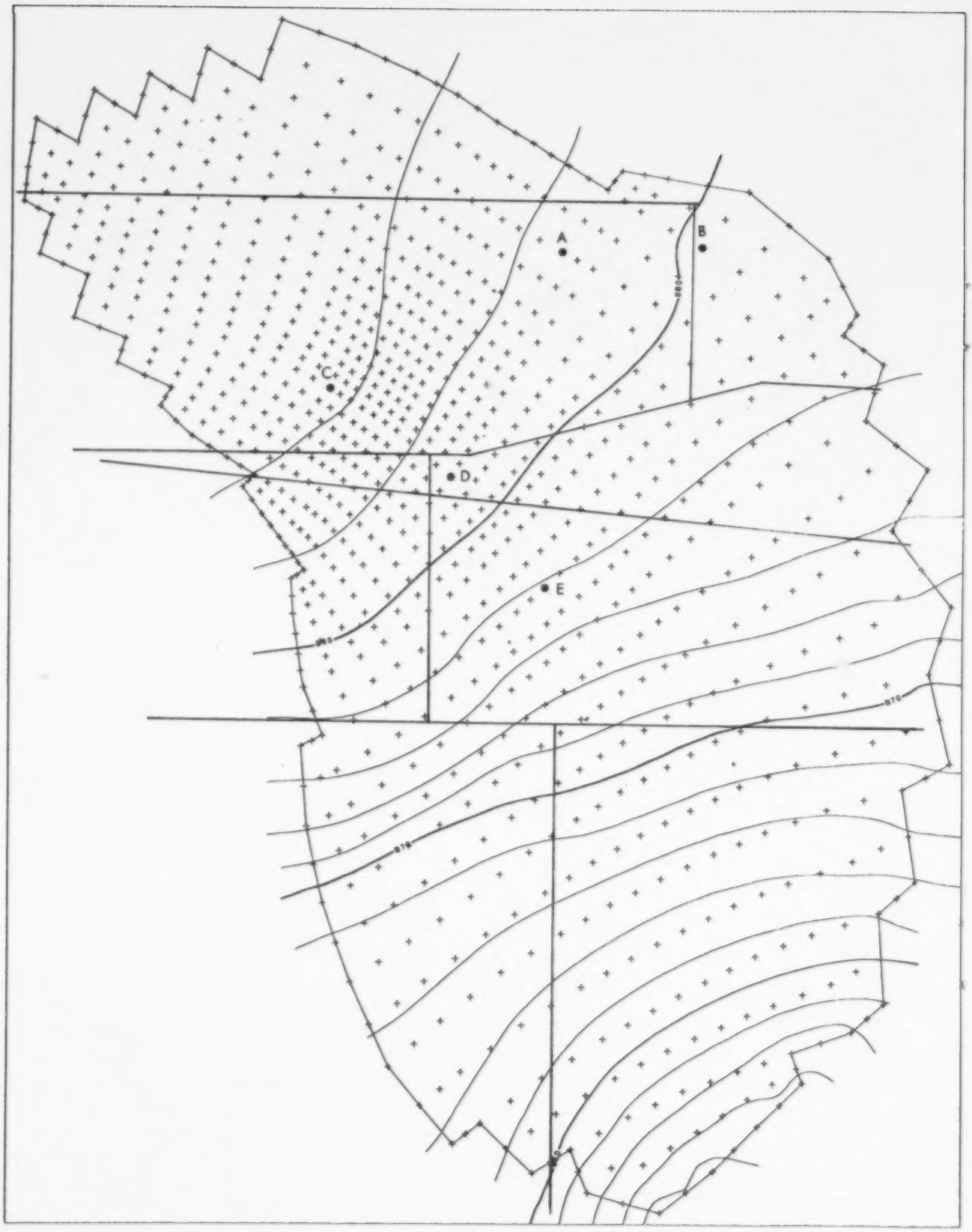


Fig. 11 Predicted piezometric contours

Fig. 12 Predicted flow vectors

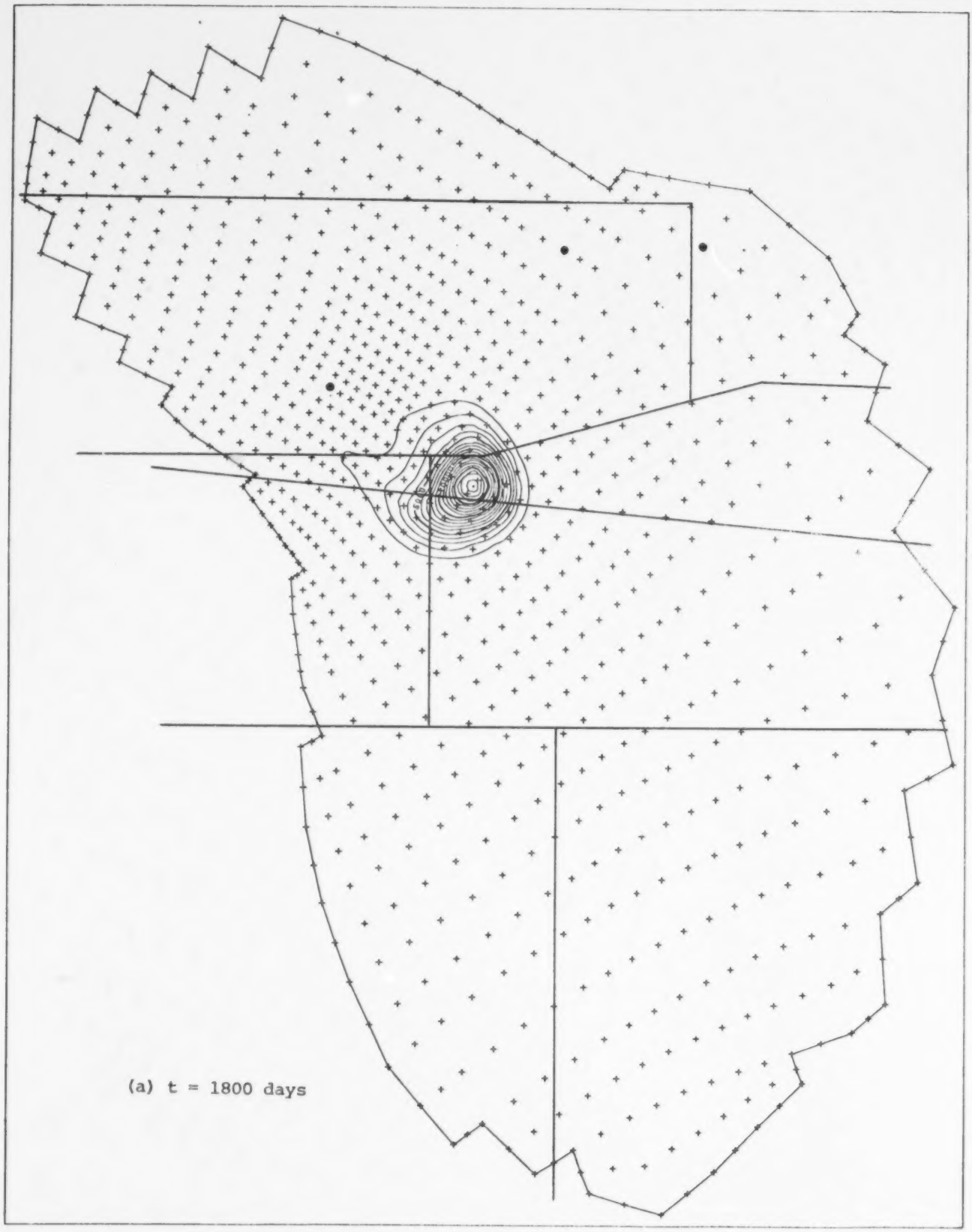


Fig. 13 Predicted concentration contours for α_L = 5 ft and α_T = 2 ft

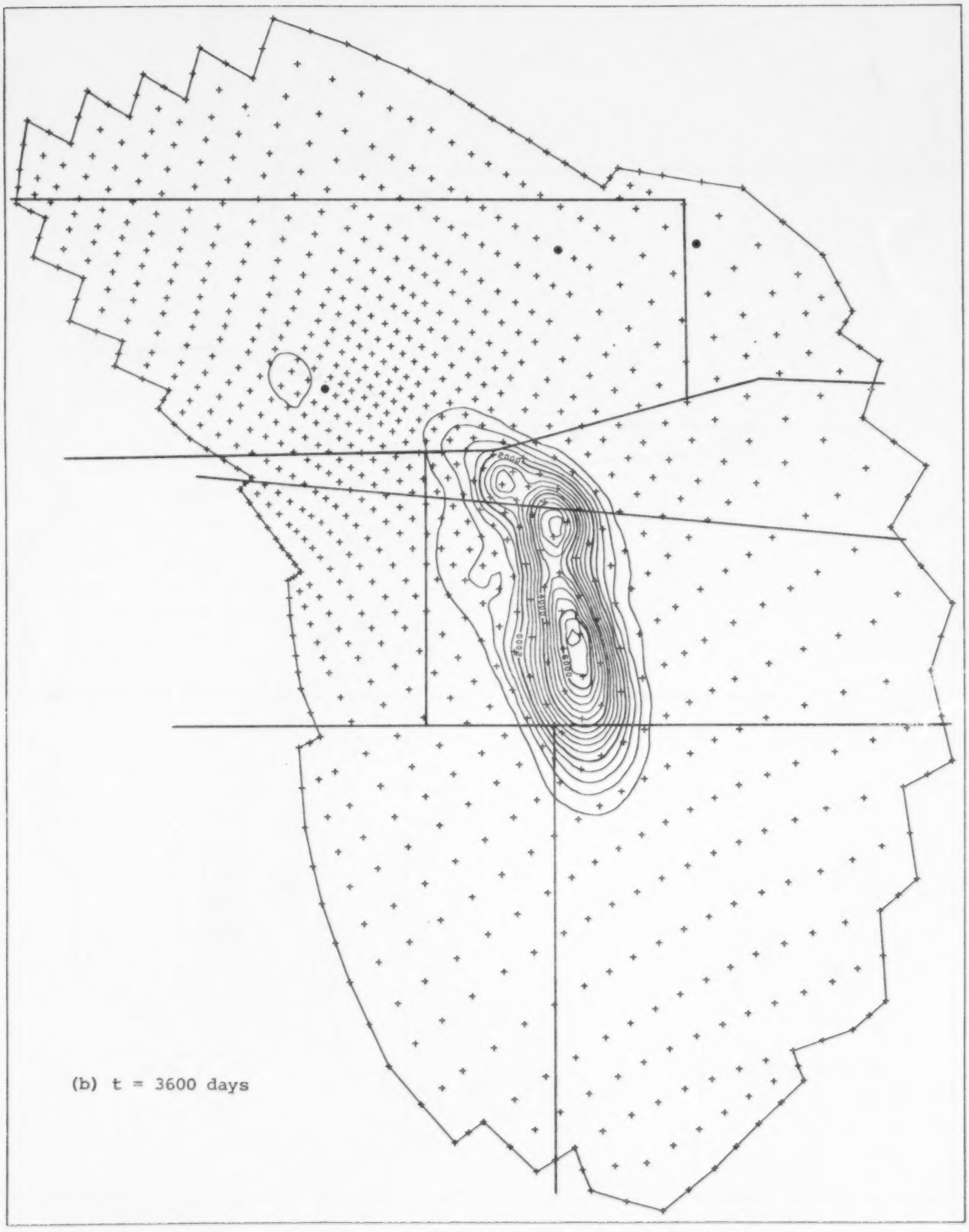


Fig. 13 (continued)

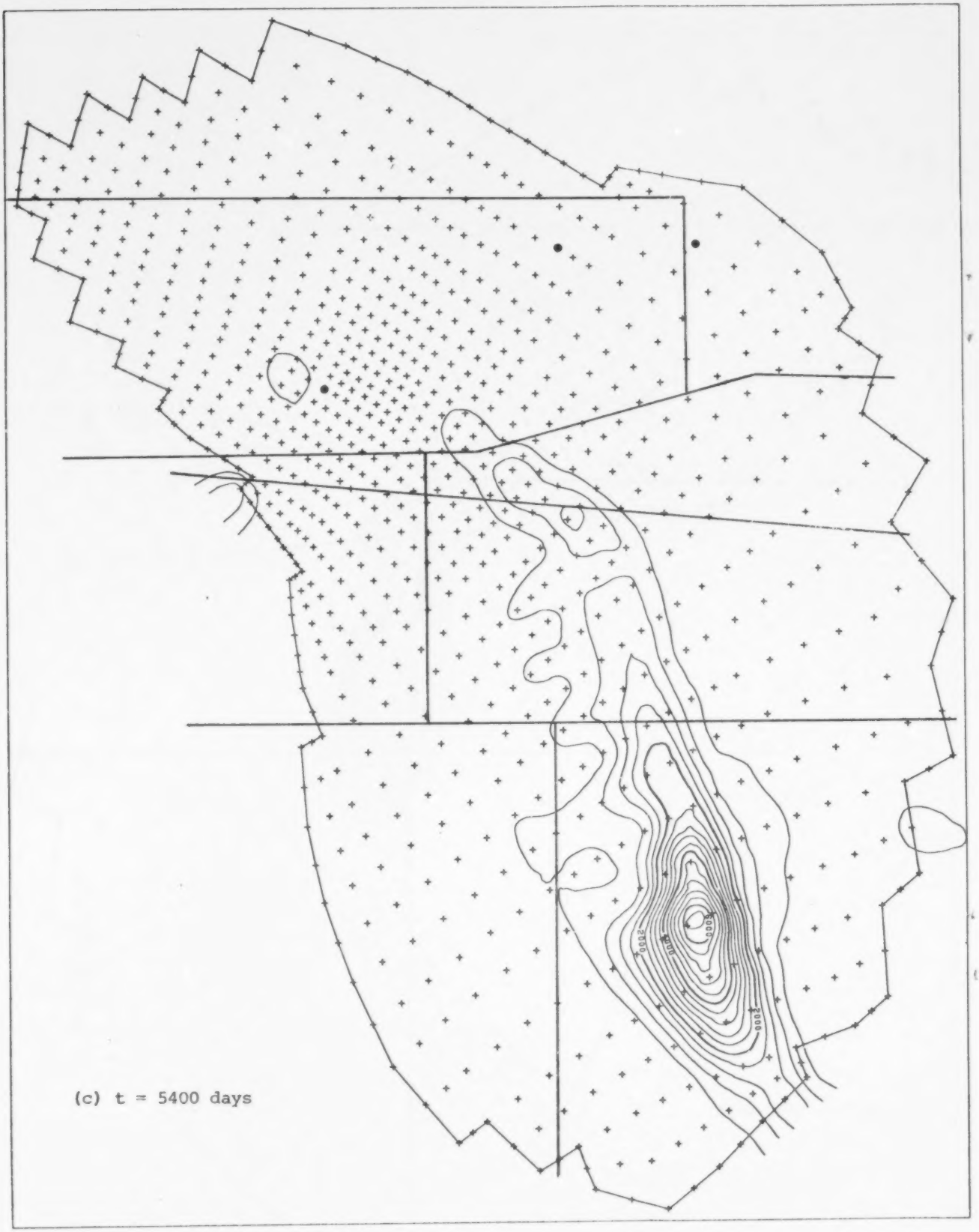
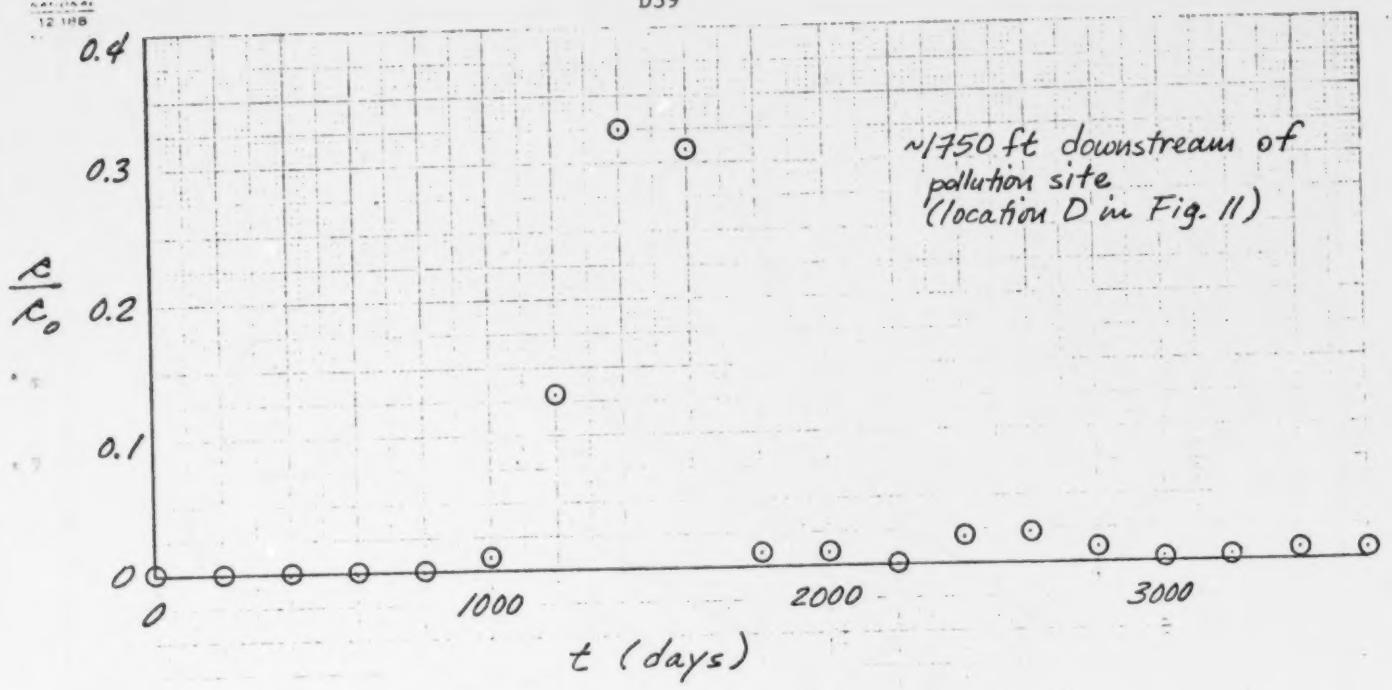


Fig. 13 (continued)



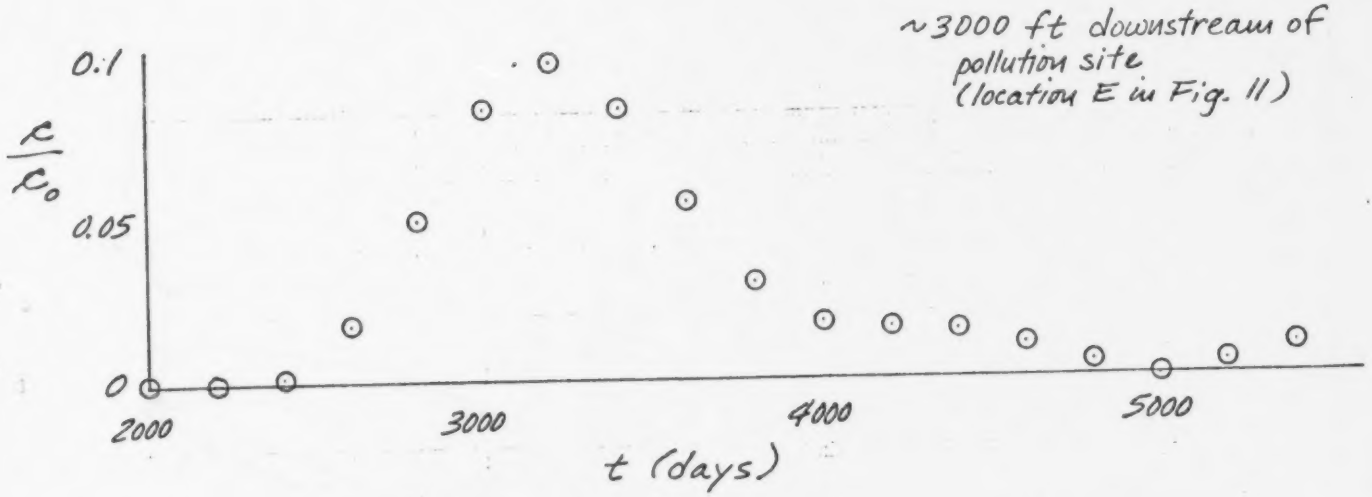


Fig. 14 Relative concentration versus time at locations D and E

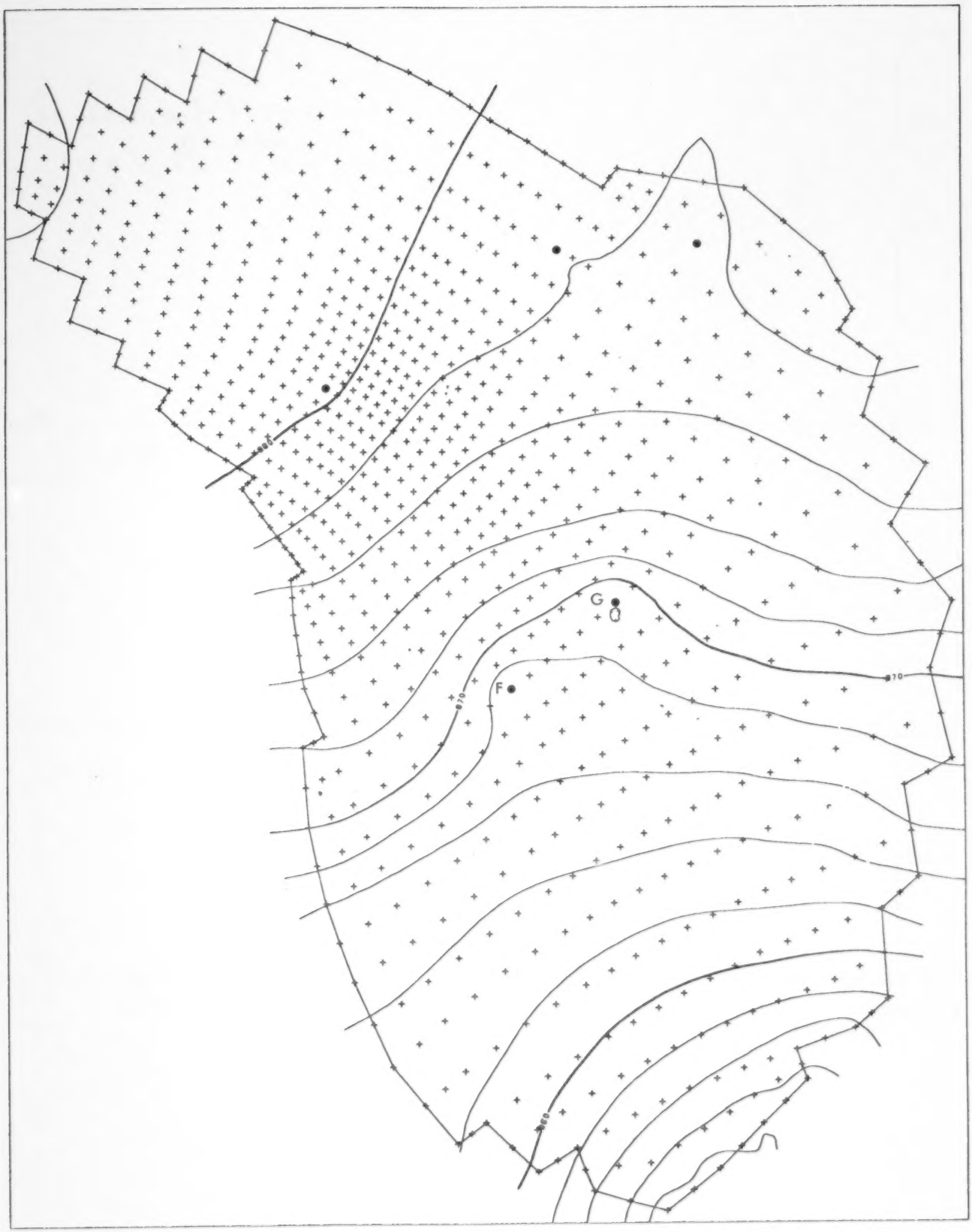


Fig. 15 Predicted piezometric contours with two purge wells

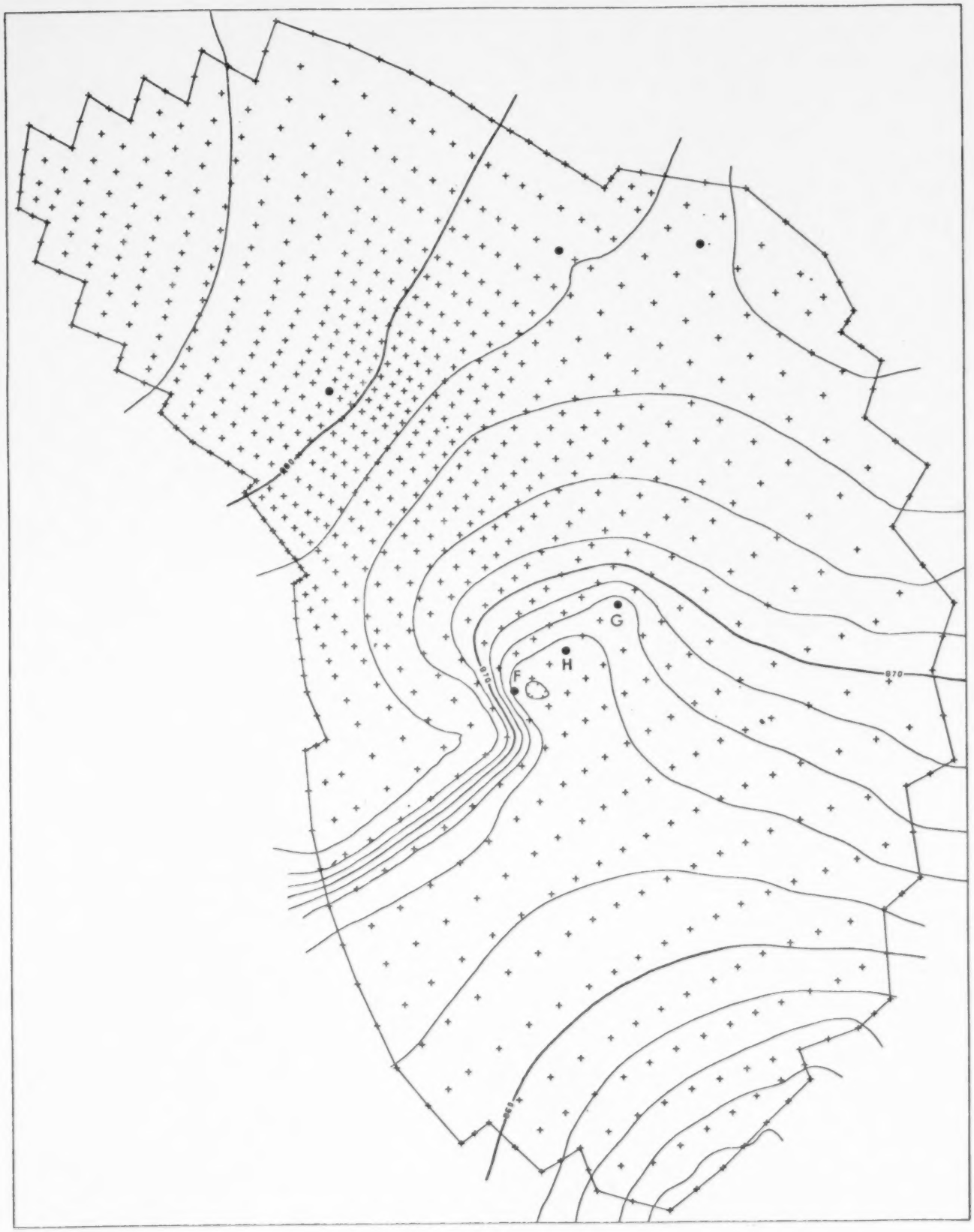


Fig. 16 Predicted piezometric contours with three purge wells